IMPROVED MATHEMATICAL TECHNIQUES

FOR SOLUTION OF ATMOSPHERIC DISPERSION MODELS

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> by Miguel T. Fleischer March, 1978

To My lovely wife, Jackie and to David and Ronnie

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CHAPTER I

INTRODUCTION

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

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

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

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

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

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

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CHAPTER II

FORMULATION OF MODELS AND THEIR SOLUTION TECHNIQUES

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

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

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

Two Dimensional-Continuous Ground Level Line Source

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

$$\frac{\partial C}{\partial t} = 0 \tag{2.2}$$

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

$$\frac{\partial}{\partial y} \left(K_y \frac{\partial C}{\partial y} \right) = 0 \tag{2.3}$$

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

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

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

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

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

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

with boundary conditions

- $C \rightarrow 0$ as $x, z \rightarrow \infty$ (2.7a)
- $C \rightarrow \infty$ at x = z = 0 (2.7b)

$$K_z \frac{\partial C}{\partial z} \neq 0$$
 as $z \neq 0, x > 0$ (2.7c)

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

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

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

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

$$C(x,z) = \frac{Qr}{u_1\Gamma(s)} \left[\frac{u_1}{r^2 K_1 x}\right]^s \exp\left(-\frac{u_1 z^2}{r^2 K_1 x}\right)$$
(2.9)

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

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

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

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

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

$$u - \frac{\partial C}{\partial x} = K_z \frac{\partial^2 C}{\partial z^2}$$
(2.11)

and the analytical solution is reduced to

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

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

$$K_z \frac{\partial C}{\partial z} = 0$$
 at $z = z_{max}$ (2.13)

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

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

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

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

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

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

$$C = \begin{cases} C_{0} & \text{at} & x = 0 \\ 0 & \text{elsewhere} \end{cases}$$
(2.16)

where C_0 is an equivalent source concentration to be calculated from the emission rate using quadrature weights. Orthogonal collocation was the numerical technique used for solving the partial differential equation (2.1). One of the reasons as to why this was done is the attractive feature of being able to position the point source exactly as a collocation point with concentration C_0 and the rest of the collocation points at x=0 with zero concentration. However, this procedure gives rise to several problems:

1) Global collocation must be used, i.e., collocate points to reduce the partial differential equation to a system of ordinary differential equations throughout the entire region of interest. Since the solution to a dispersion model should have approximately the shape of a conical plume, only a few points would be within this region. This means that at several positions in the x-direction, especially close to the source, only some points would have a certain concentration value and the rest would contain zero concentration. Accurate interpolation from such a concentration distribution is impossible;

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

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

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

A point source, which usually represents a stack, can be considered as a very small area normal to u with a concentration C_0 equivalent to the constant emission rate, as shown in Figure 2.1.

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

 $C^{i} = \begin{cases} C_{0} & \text{at } \xi=0 , \quad 0 \leq z^{*} \leq \beta \\ & & & \\ 0 & \text{at } \xi=0 , \quad z^{*} > \beta \end{cases}$ (2.17)

where C_0 can be calculated using equation (2,10):

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

$$Q = \int_{0}^{\beta} u C_{0} z_{max} dz^{*}$$

Solving for C_o;

$$C_{o} = \frac{Q}{u \beta z_{max}}$$
(2.18)

Determination of the concentration distribution as a function of the spatial variables x and z requires then the solution of equation (2,11) with boundary conditions given by (2.7c) and (2.13), and the initial condition given by (2.17). The way this model is formulated overcomes

the restrictions, 2) and 3), previously discussed,

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

$$z^{*} = (\delta_{1} + \delta_{2})\zeta + \beta - \delta_{1}$$
 (2.19)

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

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

where

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

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

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

The calculational procedure is as follows: at any integration step, the concentrations at $\zeta=0$ and $\zeta=1$ are compared with C_0 and zero, respectively. If the comparisons agree, as it is shown in Figure 2.2 the values for δ_1 and δ_2 are assumed correct and the integration continues to the next step.

Since the concentrations should approach C_0 and 0 at $\zeta=0$ and $\zeta=1$, respectively, the use of the following boundary conditions is valid:

$$\frac{\partial C}{\partial \zeta} = 0$$
 at $\zeta=0, \zeta=1$ (2.22)

If at any step, the concentration at $\zeta=0$ is considerably smaller than C_0 , δ_1 is increased and the integration is performed for that same x with the previous good solution as initial condition. This comparison stops when δ_1 becomes β . When the concentration at $\zeta=1$ is considerably larger than zero, the same previous procedure is applied to δ_2 . Finally, if an inversion layer is reached ($\delta_2=1-\beta$) global collocation is used to continue the calculations until $x=x_{max}$. In any problem β is usually small so that the condition $\delta_1=\beta$ will always be obtained before $\delta_2=1-\beta$.

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

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



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

points, equation (2,20) remains as

$$R_{1} \frac{dC_{\ell}}{d\xi} = R_{5} \sum_{i=1}^{N_{z}+2} B_{\ell i}C_{i} , \text{ for } \ell=2,\ldots,N_{z}+1$$
 (2.23)

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

$$N_{z}^{+2}$$

$$\Sigma A_{1,i}C_{i} = 0 \quad \text{at} \quad \zeta=0$$

$$N_{z}^{+2}$$

$$\Sigma A_{N_{z}^{+2},i}C_{i} = 0 \quad \text{at} \quad \zeta=1$$

$$(2.24)$$

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

$$C_{1} = -\frac{\sum_{i=2}^{N_{z}+1} A1(i)C_{i}}{A_{1,1}}$$

$$N_{z}+1$$
(2.25)

$$C_{N_{z}+2} = \frac{\sum_{i=2}^{z} A^{2}(i)C_{i}}{DEN}$$
(2.26)

where

.

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

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

$$DEN = A_{N_{z}+2,1}A_{1,N_{z}+2} - A_{1,1}A_{N_{z}+2,N_{z}+2}$$
(2.29)

Finally, by substituting equations (2,25) and (2,26), equation (2.23) in matrix notation remains as follows:

$$\frac{\mathrm{d}\mathbf{C}}{\mathrm{d}\boldsymbol{\xi}} = \mathbf{E} \mathbf{C} \tag{2.30}$$

where the elements of the matrix E are

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

The solution of equation (2.30) is given by:

$$\underline{C}(\xi) = \underline{\underline{V}} \exp \left(\underline{\underline{\Lambda}}\xi\right)\underline{\underline{U}}^{-1}\underline{\underline{C}}^{1}(\xi-\Delta\xi)$$
(2.32)

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

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

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

$$Q_{x} = \int_{0}^{z_{max}} u C(x,z) dz$$
 (2.33)

Transformation of the spatial variables gives

$$Q_{\rm x} = \int_0^1 u \ C(\xi, z^*) z_{\rm max} \ dz^*$$
 (2.34)

By substituting equation (2.19) one obtains

$$Q_{x} = \int_{0}^{\beta-\delta_{1}} u C_{0} z_{\max}^{} d\zeta + \int_{\beta-\delta_{1}}^{\beta+\delta_{2}} u C(\xi,\zeta) z_{\max}^{} d\zeta \qquad (2.35)$$

Finally, using Gaussian quadrature weights, equation (2,35) can be transformed to

$$Q_{x} = Q_{x}^{1} + uz_{max}(\delta_{1} + \delta_{2}) \sum_{i=1}^{\Sigma} W_{i}C_{i}$$
(2.36)

where

$$Q_{\mathbf{x}}^{1} = \begin{cases} u z_{\max}(\beta - \delta_{1})C_{0} & \text{for } \delta_{1} < \beta \\ 0 & \text{for } \delta_{1} = \beta \end{cases}$$
(2.37)

Two Dimensional-Continuous Elevated Line Source

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

 $C \rightarrow \infty$ at x = 0 and z = H (2.38)

The analytical solution to this problem is given by

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

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

$$C^{i} = \begin{cases} C_{0} & \text{at } \xi = 0 , h - \beta \leq z^{*} \leq h + \beta \\ 0 & \text{at } \xi = 0 , \text{ elsewhere} \end{cases}$$
(2.40)

with

$$h = \frac{H}{z_{max}}$$
(2.41)

and

$$C_{o} = \frac{Q}{2u\beta z_{max}}$$
(2.42)



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

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

$$z^{*} = (\delta_{1} + \delta_{2} + 2\beta)\zeta + h - (\beta + \delta_{1})$$
(2.43)

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

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

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

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

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

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

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

$$Q_{x} = u z_{max}^{2\beta+\delta_{1}+\delta_{2}} \sum_{i=1}^{N_{z}+2} W_{i}C_{i}$$
(2.45)



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

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Two Dimensional Models with Chemical Reactions

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

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

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

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

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

The elements of the collocation matrix would now be given by

$$E_{\ell i} = -\frac{R_5 B_{\ell,1} A_1(i)}{R_1 A_{1,1}} + \frac{R_5 B_{\ell i}}{R_1} + \frac{R_5 B_{\ell,N_2} + 2^{A2(i)}}{R_1 DEN} - \frac{k_1}{R_1} \delta_{\ell i}$$
(2.48)

where $\boldsymbol{\delta}_{\texttt{li}}$ is the Knonecker delta function,

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

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

The check on the parameter δ_1 must be performed with another criteria, i.e., if $\delta_1 < \beta$, the calculated concentration at $\zeta = 0$ should be compared to $C_0 \exp(-\frac{k_1 x}{u})$. The reason being the disappearance of contaminant due to the chemical reaction.

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

$$Q_{x} = \int_{0}^{\beta-\delta_{1}} \frac{-\frac{k_{1}\xi}{R_{1}}}{uC_{0}e} z_{max}^{\beta+\delta_{1}} d\zeta + \int_{\beta-\delta_{1}}^{\beta+\delta_{1}} \frac{uC(\xi,\zeta)z_{max}}{uC(\xi,\zeta)z_{max}} d\zeta$$
(2.50)

Therefore, equation (2.36) would contain,

$$Q_{x}^{1} = \begin{cases} uz_{\max}^{(\beta-\delta_{1})C_{0}e} & \text{for } \delta_{1} < \beta \\ 0 & \text{for } \delta_{1} = \beta \end{cases}$$

$$(2.51)$$

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

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

Three Dimensional-Continuous Point Source

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

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

At an early stage, observations of diffusion implied a dependence of K_y on the distance of travel [14]. On the grounds that it is physically irrational to regard K_y as a function of horizontal position, one approach

has been to seek solutions with K_y , as well as K_z and u, a function of height above the ground, i.e.,

$$u = u(z)$$
; $K_y = K_y(z)$; $K_z = K_z(z)$ (2.53)

For this case, equation (2.52) remains as,

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

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

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

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

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

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

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

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

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

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

 $\frac{\partial C}{\partial n} = 0 \qquad \text{at} \qquad n=0,1 \qquad (2.58)$

$$\frac{\partial C}{\partial \zeta} = 0$$
 at $\zeta=0,1$ (2.59)

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

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

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

Constant Mean Wind Velocity and Turbulent Diffusivities

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

$$R_{1} \frac{\partial C}{\partial \xi} = R_{5} \frac{\partial^{2} C}{\partial \eta^{2}} + R_{6} \frac{\partial^{2} C}{\partial \zeta^{2}} + R(C)$$
(2.60)

where

$$R_1 = \frac{u}{x_{max}}$$
(2.61)

$$R_{5} = \frac{K_{y}}{y_{max}^{2}(\delta_{1y}+\delta_{2y})^{2}}$$
(2.62)

$$R_{6} = \frac{K_{z}}{z_{max}^{2} (\delta_{1z} + \delta_{2z} + 2\beta_{z})^{2}}$$
(2.63)

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

$$R_{1} \frac{dC_{k\ell}}{d\xi} = R_{5} \sum_{i=1}^{N_{y}+2} B_{ki}^{(2)}C_{i\ell} + R_{6} \sum_{i=1}^{N_{z}+2} B_{\ell i}^{(3)}C_{ki} + R(C_{k\ell})$$
(2.64)

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

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

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

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

$$N_{y}^{+2} = X_{1,i}^{(2)} C_{il} = 0 \quad \text{at} \quad \eta = 0$$

$$N_{y}^{+2} = X_{N_{y}^{+2},i}^{(2)} C_{il} = 0 \quad \text{at} \quad \eta = 1$$

$$(2.65)$$

$$M_{y}^{+2} = X_{N_{y}^{+2},i}^{(2)} C_{il} = 0 \quad \text{at} \quad \eta = 1$$

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

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

$$C_{N_{y}+2,\ell} = \frac{\sum_{i=2}^{N_{y}+1} A_{2Y(i)}C_{i\ell}}{DENY}$$
(2.67)

where

AlY(i) =
$$A_{1,i}^{(2)} + \frac{A_{1,N_y^{+2}}^{(2)} A2Y(i)}{DENY}$$
 (2.68)

$$A2Y(i) = A_{1,1}^{(2)}A_{N_y+2,i}^{(2)} - A_{N_y+2,1}^{(2)}A_{1,i}^{(2)}$$
(2.69)

DENY =
$$A_{N_y+2,1}^{(2)} A_{1,N_y+2}^{(2)} - A_{1,1}^{(2)} A_{N_y+2,N_y+2}^{(2)}$$
 (2.70)

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

$$N_{z}^{+2} \sum_{i=1}^{N} A_{1,i}^{(3)} C_{ki} = 0 \quad \text{at} \quad \zeta=0$$
(2.71)

$$N_{z}^{+2}$$

$$\sum_{i=1}^{\Sigma} A_{z}^{(3)} C_{ki} = 0 \quad \text{at} \quad \zeta=1$$

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

$$C_{k,1} = -\frac{\sum_{i=2}^{N_{z}+1} \sum_{i=2}^{X_{i} (i) C_{ki}}}{A_{1,1}^{(3)}}$$
(2.72)
$$C_{k,N_{z}+2} = \frac{\sum_{i=2}^{N_{z}+1} \sum_{DENZ}^{X_{i} (i) C_{ki}}}{DENZ}$$
(2.73)

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

$$A2Z(i) = A_{1,1}^{(3)}A_{N_{z}+2,i}^{(3)} - A_{N_{z}+2,1}^{(3)}A_{1,i}^{(3)}$$
(2.75)

DENZ =
$$A_{N_z+2,1}^{(3)} A_{1,N_z+2}^{(3)} - A_{1,1}^{(3)} A_{N_z+2,N_z+2}^{(3)}$$
 (2.76)

Substituting equations (2.66), (2.67), (2.72), and (2.73) into equation (2.64) one obtains,
$$R_{1} \frac{dC_{k\ell}}{d\xi} = R_{5} \begin{pmatrix} N_{y}^{+1} \\ \Sigma \\ i=2 \end{pmatrix} (-B_{k,1}^{(2)} \frac{A1Y(i)}{A_{1,1}^{(2)}} + B_{ki}^{(2)} + B_{k,N_{y}^{+2}}^{(2)} \frac{A2Y(i)}{DENY})C_{i\ell} + R_{6} \begin{pmatrix} N_{z}^{+1} \\ \Sigma \\ i=2 \end{pmatrix} (-B_{\ell,1}^{(3)} \frac{A1Z(i)}{A_{1,1}^{(3)}} + B_{\ell i}^{(3)} + B_{\ell,N_{z}^{+2}}^{(3)} \frac{A2Z(i)}{DENZ})C_{ki} + R(C_{k\ell}) \end{pmatrix} + R(C_{k\ell})$$

$$(2.77)$$

or simplifying it:

$$\frac{dC_{k\ell}}{d\xi} = \frac{R_5}{R_1} \begin{pmatrix} N_y^{+1} \\ \Sigma \\ i=2 \end{pmatrix} AKY(k,i)C_{i\ell} + \frac{R_6}{R_1} \begin{pmatrix} N_z^{+1} \\ \Sigma \\ i=2 \end{pmatrix} + \frac{R(C_{k\ell})}{R_1} + \frac{R(C_{k\ell})}{R_1}$$
(2.78)

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

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

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

$$C_{kl}^{i} = \begin{cases} C_{0} & \text{at} \quad \xi=0, \quad 0 \leq y^{*} \leq \beta_{y} \\ & h - \beta_{z} \leq z^{*} \leq h + \beta_{z} \\ 0 & \text{at} \quad \xi=0, \quad y^{*} > \beta_{y} \\ & \text{elsewhere } z^{*} \end{cases}$$

$$(2.79)$$

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

$$Q = 2 \int_{0}^{\beta} \int_{\beta_{z}}^{\beta_{z}} u(h) C_{0} y_{max} dy^{*} z_{max} dz^{*}$$
(2.80)

Solving for C_0 , the equivalent concentration at the source one obtains,

$$C_{o} = \frac{Q}{4u(h)\beta_{z}^{z}\max^{g}y^{y}\max}$$
(2.81)

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

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

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

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

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complexity of the present air pollution model requires a large number of differential equations to be solved. The use of both methods involved a large computational time.

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

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

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

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

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

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

$$Q_{x} = 2 \int_{0}^{y_{max}} \int_{0}^{z_{max}} u C(x,y,z) dy dz$$
 (2.84)

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

$$Q_{x} = 2u(\delta_{1y} + \delta_{2y})y_{\max}(\delta_{1z} + \delta_{2z} + 2\beta_{z})z_{\max} \sum_{k=1}^{N_{y}+2} \sum_{\ell=1}^{N_{z}+2} w_{k}^{(2)}w_{\ell}^{(3)}C_{k\ell}$$
(2.85)

Variable Mean Wind Velocity and Turbulent Diffusivities

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

$$R_{1}(\zeta) \frac{\partial C}{\partial \xi} + R_{3}(\zeta) \frac{\partial C}{\partial \zeta} = R_{5}(\zeta) \frac{\partial^{2} C}{\partial \eta^{2}} + R_{6}(\zeta) \frac{\partial^{2} C}{\partial \zeta^{2}} + R(C)$$
(2.86)

where

$$R_{1}(\zeta) = \frac{u(\zeta)}{x_{max}}$$
(2.87)

$$R_{3}(\zeta) = -\frac{\frac{dK_{z}}{dz}(\zeta)}{z_{max}(\delta_{1z}+\delta_{2z}+2\beta_{z})}$$
(2.88)

$$R_{5}(\zeta) = \frac{K_{y}(\zeta)}{y_{\max}^{2}(\delta_{1y}+\delta_{2y})^{2}}$$
(2.89)

$$R_{6}(\zeta) = \frac{K_{z}(\zeta)}{z_{\max}^{2}(\delta_{1z}+\delta_{2z}+2\beta_{z})^{2}}$$
(2.90)

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

$$\frac{dC_{k\ell}}{d\xi} = -\frac{R_{3}(\ell)}{R_{1}(\ell)} \begin{pmatrix} N_{z}^{+1} \\ \Sigma \\ i=2 \end{pmatrix} DAKZ(\ell,i)C_{ki} \end{pmatrix} + \frac{R_{5}(\ell)}{R_{1}(\ell)} \begin{pmatrix} N_{y}^{+1} \\ \Sigma \\ i=2 \end{pmatrix} AKY(k,i)C_{i\ell} \end{pmatrix} + \frac{R_{6}(\ell)}{R_{1}(\ell)} \begin{pmatrix} N_{z}^{+1} \\ \Sigma \\ i=2 \end{pmatrix} AKZ(\ell,i)C_{ki} \end{pmatrix} + \frac{R(C_{k\ell})}{R_{1}(\ell)}$$
(2.91)
for k=2,...,N_y+1
$$\ell=2,...,N_{z}^{+1}$$

where

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

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

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

$$Q_{x} = 2(\delta_{iy} + \delta_{2y})y_{max}(\delta_{1z} + \delta_{2z} + 2\beta_{z})z_{max}\sum_{k=1}^{N_{y}+2} u(\ell)W_{k}^{(2)}W_{\ell}^{(3)}C_{k\ell}$$
(2.93)

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

Three Dimensional Mean Wind Velocity

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

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

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

$$u=u(z); v=v(z); K_y=K_y(z); K_z=K_z(z)$$
 (2.95)

equation (2.94) remains as

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

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

$$y^* = \frac{\frac{y}{y_{\text{max}}} + 1}{2}$$
(2.97)

$$z^* = \frac{z}{z_{\text{max}}}$$
(2.98)

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

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

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

The initial condition for this case can then be stated as

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

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

$$R_{1}(\zeta) \frac{\partial C}{\partial \xi} + R_{2}(\zeta) \frac{\partial C}{\partial \eta} + R_{3}(\zeta) \frac{\partial C}{\partial \zeta} = R_{5}(\zeta) \frac{\partial^{2}C}{\partial \eta^{2}} + R_{6}(\zeta) \frac{\partial^{2}C}{\partial \zeta^{2}} + R(C) \quad (2.102)$$

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

$$R_{2}(\zeta) = \frac{v(\zeta)}{2y_{\max}(\delta_{1y} + \delta_{2y} + 2\beta_{y})}$$
(2.104)

$$R_{3}(\zeta) = -\frac{\frac{dK_{z}}{dz}(\zeta)}{z_{max}(\delta_{1z}+\delta_{2z}+2\beta_{z})}$$
(2.105)

$$R_{5}(\zeta) = \frac{K_{y}(\zeta)}{4y_{\max}^{2}(\delta_{1y}+\delta_{2y}+2\beta_{y})^{2}}$$
(2.106)

$$R_{6}(\zeta) = \frac{K_{z}(\zeta)}{z_{\max}^{2}(\delta_{1z} + \delta_{2z} + 2\beta_{z})^{2}}$$
(2.107)

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

$$-\frac{R_{2}(l)}{R_{1}(l)}\begin{pmatrix}N_{y}^{+1}\\\Sigma\\i=2\end{pmatrix}$$
(2.108)

with

$$AVY(k,i) = -A_{k,1}^{(2)} \frac{AIY(i)}{A_{1,1}^{(2)}} + A_{ki}^{(2)} + A_{k,N_y}^{(2)} + \frac{A2Y(i)}{DENY}$$
(2.109)

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

$$C_{0} \quad \text{at} \quad \xi=0, \quad \frac{1}{2} - \beta_{y} \leq y^{*} \leq \frac{1}{2} + \beta_{y}$$

$$C_{kl}^{i} = \begin{cases} \qquad h - \beta_{z} \leq z^{*} \leq h + \beta_{z} \end{cases}$$

$$(2.110)$$

$$0 \quad \text{at} \quad \xi=0, \quad \text{elsewhere } y^{*} \text{ and } z^{*}$$

The equivalent source concentration can again be obtained using continuity:

$$Q = \int_{-\beta_{y}}^{\beta_{y}} \int_{-\beta_{z}}^{\beta_{z}} u(h) C_{0}(2y_{max}dy^{*}) z_{max}dz^{*}$$
(2.111)

Solving for C_0 , one obtains

$$C_{o} = \frac{Q}{8u(h)y_{max}^{\beta}y^{z}_{max}^{\beta}z}$$
(2.112)

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

$$Q_{x} = \int_{-y_{max}}^{y_{max}} \int_{0}^{z_{max}} u(z)C(x,y,z)dydz$$
(2.113)

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

$$Q_{x} = 2(\delta_{1y} + \delta_{2y} + 2\beta_{y})y_{max}(\delta_{1z} + \delta_{2z} + 2\beta_{z})z_{max} \sum_{k=1}^{N_{y}+2} u(\ell)W_{k}^{(2)}W_{\ell}^{(3)}C_{k\ell}$$
(2.114)

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

$$R_{3}(\zeta) = \frac{w(\zeta) - \frac{dK_{z}}{dz}(\zeta)}{z_{\max}(\delta_{1z} + \delta_{2z} + 2\beta_{z})}$$
(2.115)

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

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

CHAPTER III

PARAMETERS ESTIMATION

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

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

$$e = \left(\frac{\frac{C}{a} - C}{C_{a}}\right) 100 \qquad (\%) \qquad (3.1)$$

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

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

Mathematical Parameters

Two Dimensional-Continuous Ground Level Line Source

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



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

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

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

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

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

As it was expected, as N increases the error decreases and the computer time increases. The differences in the computer time spent are not very large with the exception of the last two cases, N=8 and N=10. In addition, the error is greatly minimized as N increases from 4 to 8 interior points, but the difference between the last two cases is negligible. Therefore, the number of interior orthogonal collocation points selected is 8. The next parametric study done, on β , is shown in Figure 3.2. For this case, r was again given an arbitrary value of 0.01. Time requirements are given in Table 3.2.

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

β	Time (sec)
.003	31
.006	26
.018	32

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

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



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

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

^{\$} 2	Q _x (gm/m s)
.004	.9
.006	1.1
.005	1.0

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



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

Table 3.4	Computer	Time	requiremen	ts for	Paramet	ric
	Study on	r - (Ground Leve	1 Line	Source	Mode1

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

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

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

Table 3.5 Computer Time Requirements for Parametric

Study	on	^z max	-	Ground	Level	Line	Source	Mode1
-------	----	------------------	---	--------	-------	------	--------	-------

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

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

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



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

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

Two Dimensional - Continuous Elevated Line Source

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

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

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

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



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

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

A value of 0,0012 was assigned for β in this model. The same procedure as before was used to estimate the parameters δ_1 and δ_2 . For an emission rate of 1 gm/s m, Table 3.7 shows the final values for δ_1 and δ_2 obtained.

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

δ ₁	^δ 2	Q _x (gm/s)
.0030	.0030	1.0343
.0026	.0026	.9358
.002861	.002861	1.0001

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

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

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

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

Three Dimensional Continuous Point Source

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

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



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

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

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

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

Table 3.9 Mass Flux vs δ_{2v} at the First Integration

Step - Elevated Point Source Model

^{\$} 2y	Q _x (kg/s)
.01	.95607
.011	1,01981
.01069	1,00005

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

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

Table 3.10 Computer Time Requirements for Parametric

ε	Time (sec)
1x10 ⁻⁵	180
1×10^{-6}	190
1×10^{-7}	200
1x10 ⁻⁸	290

Study on ε - Elevated Point Source Model

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



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

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

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

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

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

ε	Time (sec)
1x10 ⁻⁵	250
1×10^{-6}	260
1×10^{-7}	270
1×10^{-8}	310

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Since there was no dependence of ε in the error for this case, a parametric study to check r was performed again, and is shown in Figure 3.8. It can be seen that the absolute error is indeed decreased by using a smaller stepsize, and the peak is converted to a damped curve at downwind distances close to the point source. As expected and discussed before, as the ratio increased the error increased and the computer time decreased to 250 seconds ($\varepsilon = 1 \times 10^{-7}$). The main objective of the present work is to develop a highly accurate method of solution, so the small stepsize was adopted with an upper error bound of $\varepsilon = 1 \times 10^{-7}$.

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

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



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

Meteorological Parameters

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

Turbulent Diffusivities K, K

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

Among the best of these works, Eschenroeder and Martinez [5] relate K_z to elevation and most importantly to stability classes, as defined by Pasquill and Gifford [18], a parameter that is widely used and known. The trapezoidal profile for K_z , discussed by Fleischer [8], and the values for the maximum constant vertical diffusivities from the knee height up to the inversion layer seem to describe fairly well K_z . Eschenroeder and Martinez, based on a Los Angeles tetroon data, assigned a value of 500 m²/s for the constant horizontal diffusivity. Unfortunately, this large value, when compared to others, is not appropriate to use as a typical measure for K_y . Therefore, their description for K_z is used in the present work, but with different absolute values for K_z and K_y .

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

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

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

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FIGURE 3.10 COMPARISON OF DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL WITH ANALYTICAL SOLUTION AND GAUSSIAN PLUME EQUATION - STABILITY CLASS B -63-


FIGURE 3.11 COMPARISON OF DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL WITH ANALYTICAL SOLUTION AND GAUSSIAN PLUME EQUATION - STABILITY CLASS C -64



FIGURE 3.12 COMPARISON OF DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL WITH ANALYTICAL SOLUTION AND GAUSSIAN PLUME EQUATION - STABILITY CLASS D -65-



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



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

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

It should be pointed out that the present mathematical technique is valid for any type of relationship between the turbulent diffusivities and meteorological and/or spatial variables. The more complicated models are compared to the Gaussian plume equation in Chapter IV. The selection of the present procedure to determine the turbulent diffusivities was done in order to present meaningful comparisons besides lack of a reasonable algorithm. The results for the constant vertical and horizontal diffusivities obtained are presented in Table 3,12.

Table 3.	12 Cons ⁻	tant Ti	irbule	ent	Diff	fusivitie	es	and
	Wind	Speed	used	in	the	Present	Me	thod

Stability Class	Wind Speed (m/s)	(m^2/s)	Ky (m ² /s)
A	2	11	18,15
В	3	10,75	25.26
С	5	10.5	30.76
D	6	5,2	46.28
Е	3	1.5	30,00
F	2	.325	22.75

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

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



FIGURE 3.15 VERTICAL DIFFUSIVITY PROFILES IN THE PRESENT WORK

Velocity Profile

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

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

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

Table 3.13 Estimates for the Parameters

in Equation (3.2)

Stability Class	m	u ₁ (z ₁ =10m) (m/s)		
A	.02	2		
D	.14	6		
F	.83	2		

At some elevation z_G called the geostrophic elevation, which is determined in the following two-dimensional wind velocity description,

the mean wind velocity should become constant. Therefore, the complete specification for the one-dimensional mean wind velocity is given by

$$u = u_{10} (\frac{z}{10})^{m}$$
 $0 < z < z_{G}$ (3.3)

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

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

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

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

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

where $f = 2w \sin \phi \approx 1.458 \times 10^{-4} \sin \phi \frac{1}{\sec}$ and is called the Coriolis parameter, w being the angular velocity of rotation of the earth and ϕ the geographical latitude.

By assuming that the eddy stresses are

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

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

equations (3.5) and (3.6) become

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

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

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

$$f u_{G} = -\frac{1}{\rho} \frac{\partial p}{\partial y}$$
(3.11)

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

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

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

$$v = u_{G} e^{-az} \sin az$$
 (3.13)

where

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

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

$$z'_{\rm G} = \frac{\pi}{a} \tag{3.15}$$

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

Table 3.14 Geostrophic Elevations used

in the Present Work

_	ability Class	z _G (m)
	A	1475
	В	1455
	С	1440
	D	1015
	Ε	545
	F	255

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

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

Stability Class	α(°)
A	42
В	42
С	42
D	41
E	37
F	29

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

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

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

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

$$v = u_{G}e^{-az} \sin az$$
 for $\Delta < z < z_{G}$ (3.19)

$$v = 0$$
 for $z \ge z_G$ (3.20)

where

$$u_{50}^{c} = u_{G}(\frac{10}{50})^{m} (1 - e^{-50a} \cos 50a)$$
 (3.21)

.

is required for a continuous velocity profile.

CHAPTER IV

PRESENTATION AND ANALYSIS OF RESULTS

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

Two-Dimensional Models

. The first problem that was simulated includes pollutant removal from the atmosphere, represented by a simplified first order chemical reaction model, and applied to the continuous ground level line source case. The value of 1.67×10^{-3} per minute or 10% loss per hour was used as the reaction rate constant. The results, obtained in 27 seconds of CPU time, are presented in Figure 4.1. They indeed show that there is no need to include chemical reactions to a steady state model since the concentration values can be calculated by multiplying the analytical solution to the factor $\exp(-\frac{k_1x}{u})$. This factor is the result of the chemical reaction model when solved by itself.

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

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

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

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

Three-Dimensional Models

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

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



TWO DIMENSIONAL MODEL WITH INVERSION LAYER



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

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FIGURE 4.4 DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL - THREE DIMENSIONAL MODELS - STABILITY CLASS D -82-



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

•

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

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

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

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



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

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

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

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

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

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



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

With the present work validated for the case of a two-dimensional wind velocity profile, the next step was to solve the problem with the Coriolis effect. The wind velocity was represented by equations (3.16) through (3.21) and the vertical diffusivity profile by Figure 3.15. The constant horizontal diffusivity was given by Table 3.12. The geostrophic velocity was taken to be the same as $u_{\rm G}$ given by the power-law equation, with $u_{\rm 1}$ for a stability class D assumed to be equal to 6 m/s. A value of $u_{\rm G}$ = 11.45 m/s was calculated for these conditions.

Isopleths of 3 mg/m³ for the present model and the constant wind speed and turbulent diffusivity are shown in Figure 4.9. Both cases are quite different, as expected. The centerline for case (a) occurs at y=0 while for case (b) is skewed to the left. Furthermore, the areas are different but the mass flux is the same, i.e., 1 kg/s. The reason being that in general, the concentrations for the constant case are higher than for the Coriolis model, e.g., the maximum concentrations found were . 5.36 mg/m^3 and 5.00 mg/m^3 , respectively. The peculiar form of the curve at the left, i.e., more voluminous is due to the effect that the isopleth has reached the ground and the material is being reflected upwards.

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

-88-



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



FIGURE 4.9 ISOPLETHS AT A CONSTANT × - THREE DIMENSIONAL MODELS



FIGURE 4.10 DOWNWIND CONCENTRATION DISTRIBUTION AT GROUND LEVEL - CORIOLIS EFFECT VS GAUSSIAN PLUME EQUATION -91-

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

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

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

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Downwind Positions - Coriolis Effect

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

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

CHAPTER V

SUMMARY OF RESULTS, CONCLUSIONS AND RECOMMENDATIONS

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

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

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

Empirical equations were used to describe the mean wind velocity

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

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

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

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

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

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

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

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

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

BIBLIOGRAPHY

- Barad, M.L., "Project Prairie Grass, A Field Program in Diffusion", Vol. I, Geophysical Research Papers No. 59, AFCRC Report TR-58-235 (i) (1958).
- Barad, M.L., "Project Prairie Grass, A Field Program in Diffusion", Vol. II, Geophysical Research Papers No. 59, AFCRC Report TR-58-235 (ii) (1959).
- 3. Caillaud, J.B. and L. Padmanabhan, "An Improved Semi-Implicit Runge-Kutta Method for Stiff Systems", Chem. Eng. Journal, 2, 227 (1971).
- 4. Calder, K.L., "Multiple-Source Plume Models of Urban Air Pollution-Their General Structure", Atmospheric Environment, 11, 403 (1977).
- 5. Eschenroeder, A.Q., J.R. Martinez and R.A. Nordsieck, "Evaluation of a Diffusion Model for Photochemical Smog Simulation", General Research Corporation, EPA-R4-73-012a, October (1972).
- 6. Eskridge, R.E. and K.L. Demerjian, "Evaluation of a Numerical Scheme for Solving a Conservation of Species Equation", Proc. 1976 Summer Computer Simulation Conf., Washington, D.C., 394 (1976).
- 7. Eskridge, R.E. and K.L. Demerjian, "Evaluation of Numerical Schemes for Solving a Conservation of Species Equation with Chemical Terms", Atmospheric Environment, 11, 1029 (1977).
- 8. Fleischer, M.T., "Solution of a Generalized Air Pollution Model by Orthogonal Collocation", M.S. Thesis, Dept. of Chemical Engineering, University of Houston (1975).
- 9. Gifford, F.A., Jr., "An Outline of Theories of Diffusion in the Lower Layers of the Atmosphere", in Slade, D.H., Editor, Meteorology and Atomic Energy, USAEC, Div. Tech. Inf., Oak Ridge, Tenn. (1968).
- Haugen, D.A., "Project Prairie Grass, A Field Program in Diffusion", Vol. III, Geophysical Research Papers No. 59, AFCRC Report TR-58-235 (iii) (1959).
- IBM Application Program, "System/360 Scientific Subroutine Package", H20-0166-5, IBM Co., 6th Ed., 333 (1970).
- 12. Michelsen, M.L., "Algorithms for Collocation Solution of Ordinary and Partial Differential Equations", Instituttet for Kemiteknik (1973).

- Monin, A.S. and A.M. Yaglom, <u>Statistical Fluid Mechanics: Mechanics</u> of Turbulence, Vol. I, the M.I.T. Press, Cambridge, Mass. (1971) (English translation).
- 14. Pasquill, F., Atmospheric Diffusion, 2nd Ed., John Wiley and Sons, New York (1974).
- Rizzi, A.W. and H.E. Bailey, "Split Space-Marching Finite-Volume Method for Chemically Reacting Supersonic Flow", AIAA J., <u>14</u>, 621 (1976).
- 16. Seinfeld, J.H., Air Pollution, McGraw-Hill Book Co., New York (1975).
- 17. Sutton, O.G., Micrometeorology, McGraw-Hill Book Co., New York (1953).
- Turner, D.B., Workbook of Atmospheric Dispersion Estimates, PHS Publ. No. 999-AP-26 (1969).
- Villadsen, J.V. and M.L. Michelsen, <u>Solution of Differential</u> <u>Equation Models by Polynomial Approximation</u>, Inst. for Kemiteknik <u>Numer. Inst. Danmarks Tekniske Højskole</u>, Copenhagen (1976).
APPENDICES

APPENDIX A

COMPUTER PROGRAM LISTING

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

1:	С	*****	* * *	*****	** * №∆IN	10
2:	С				MAIN	20
3:	С	THREE DIMENSI	CNA	L MODEL WITH CORICLIS EFFECT	MAIN	30
4:	С				MAIN	40
5:	С	CEVELOPED BY I	MIG	BUEL T. FLEISCHER	MAIN	50
6:	С				MAIN	60
7:	С	****	* * *	******	***MAIN	7 J
8:	С				MAIN	80
9:	С				ΜΔΙΝ	90
10:	С	NOMENCLATURE			MAIN	100
11:	С				MAIN	110
12:	С	ΑΚΥΒ,ΑΚΖΒ	-	TURBULENT DIFFUSIVITIES	MAIN	120
13:	С	ΔLΡΗΔ		CONSTANT TO DETERMINE THE FORIZONTAL DIFFUSIVITY	MAIN	130
14:	С	ΔΜ, ΔΜΜ	-	CLNSTANTS USED IN THE VELOCITY PROFILES	NAIN	140
15:	С	BETAY, BETAZ	-	MATHEMATICAL PARAMETERS IN MCDEL	MAIN	150
16:	С	CRX	-	EQUIVALENT SCURCE CONCENTRATION	MAIN	160
17:	С	C(Y,Z)	-	MEAN CONCENTRATION AT Y AND Z	MAIN	177
18:	С	CKN(ISTB)	-	KNEE HEIGHT FOR AKZB	MAIN	180
19:	С	DUN(ISTB)	-	REFERENCE HEIGHT FOR POWER-LAW VELOCITY PROFILE	MAIN	19ι
2):	С	D1Y,,D2Z		MATHEMATICAL PARAMETERS IN MCCEL	MAIN	200
21:	С	CC1Y, ., DC2Z	-	INCREMENTS OF THE PREVIOUS PARAMETERS	MAIN	210
22:	С	HGED(ISTB)		GEOSTROPHIC ELEVATION	MAIN	220
23:	С	HSKN	-	IF GT H, NC SECOND KNEE HEIGHT FOR AKZE	MAIN	230
24:	С	ISTB		STABILITY CLASS (1 VERY UNSTABLE, 6 VERY STABLE)	MAIN	24)
25:	С	NY,NZ		NUMBER OF COLLOCATION POINTS IN Y,Z DIRECTIONS	MAIN	25 J
26:	С	Q S	-	SCURCE STRENGTH	MAIN	260
27:	С	RATIO		RATIO OF BOUNDARY TO CENTERLINF CONCENTRATION	MAIN	270
28:	С	SEL	-	EFFECTIVE EMISSION HEIGHT (LIMITS C TO 1)	MAIN	280
29:	С	L,V	-	WIND VELCCITY IN X,Y DIRECTIONS	MAIN	290
30:	С	UCR	-	VELOCITY AT GROUND LEVEL	MAIN	301
31:	С	US	-	VELOCITY AT THE EFFECTIVE EMISSION HEIGHT	MAIN	310
32:	С	LST	-	GECSTROPHIC VELOCITY	MAIN	320
33:	С	hY, WZ	-	QUADRATURE WEIGHTS	MAIN	330
34:	С	X, XA, DX	-	CUWNWIND DIRECTION, INITIAL VALUE, INCREMENT	MAIN	341
35:	С	XMAX,YMAX,H	-	MAXIMUM DISTANCES IN X,Y,Z DIRECTIONS	MAIN	353

36:	C Y	Y,Z - LATERAL AND VERTICAL DIF	ECTIENS	MAI.J	351
3/:	C			MAIN	373
38:		IMPLICII REAL*3(A-H, C-Z)		MAIN	380
39:		EXTERNAL FOI		MAIN	390
4(:		EIMENSION FAY(12), FAZ(12), FB(12), FC(1)	2), RTY(12), RTZ(12),	MAIN	4))
41:		$1 \Delta Y (12, 12), EY (12, 12), AZ (12, 12), BZ (12, 12)$	2), WY(12), WZ(12),	MAIN	417
42:		2VEC(12),A1Y(12),A2Y(12),A1Z(12),A2Z(1	2), AVY(12,12),	MAIN	42J
43:		² Y(12),Z(12),AKY(12,12),AKZ(12,12),DAH	Z(12,12),ACTY(12),ACTZ(12),	MAIN	431
44:	4	4YINTP(12),ZINTP(12),P(170),CECO(12),E	HCO(12), CECCY(12),	MAIN	44 1
45:		5C(12,12),CC(12,12),PW(107,130),		MAIN	45
46:		EPRM1(5), DY(1CC), AUX(8, 1CD), EKN(6), EUN	(5),FGFC(6),	M ∆ I^;	460
4/:		/R1(12), R2(12), R3(12), R5(12), R6(12), AK	YB(12), AKZB(12), CAKZP(12),	MAIN	47)
48:	-	8U(12),V(12)		MAIN	486
49:	C			MAIN	495
50:	C	READ AND WRITE INPUT DATA		MAIN	530
51:	C			MAIN	51)
52:		FEAD(5,135) NY,NZ,ISTR		MAIN	520
53:	140	FCRMAT(3I5)		MAIN	531
54:		READ(5,101) XMAX, H, YMAX, ALPHA, AK		MAIN	54)
55:	171	FORMAT(5D15.4)		MAIN	5うじ
56:	_	READ(5,106) UST, AM, UGR, QS, SEL		MAIN	560
57:	106	FURMAT(5D15.4)		MAIN	י 57
58:	_	READ(5,98) (DKN(I), I=1,6)		MAI.1	58.
59:	58	FORMAT(EDIC.1)		MAIN	500
60:		READ(5,99) (DUM(I), $I=1, 6$)		MAIN	693
61:		READ(5,99) (FGEC(I), I=1,6)		MAIN	61
62:	55	FURMAT(6010.1)		ΜΔΙΝ	627
63:		READ(5, 104) (PRMT(I), I=1,4)		MAIN	E3`
6 4 :	14	FORMAT(4C15.4)		MAIN	64]
65 :		PEAD(5,102) DIY,D2Y,PATIC,BETAY		MVIN	65r
66:		READ(5,1/2C) D1Z,D2Z,BFTAZ		MAIN	661
67:	1)2	FURMAT(4D15.4)		MAIN	67')
68:	1020	FORMAT(3D15.4)		MAIN	68,
69:		READ(5,103) XC, DX, DD1Y, DD2Y		NUIN	690
71:		READ(5,1,2) DD1Z,ED2Z,HSKN,AMM		NAIN	7,
71:	1 3	FORMAT(4015.4)		MAIN	71:

72:	WRITE(6,1(5) (PRMT(I), $I=1,4$)	MAIN 727
77:	1 5 FUPMAT(10(/),2CX, 'PRMTS =',4(E15.4,10X))	MAIN 737
74:	WRITE(6,4CD) XMAX,YMAX,H,SEL,UST,UGR,AM,AMM,QS,ALPHA,AK,XC,DX,	MAIN 740
75:	1RATIO, BETAY, BETAZ, DIY, DZY, DIZ, CZZ, CCIY, CC2Y, CDIZ, CC2Z, NY, NZ, ISTB,	MAIN 750
76:	2CKN(ISTB),CUN(ISTB),HSKN,HGED(ISTB)	MAIN 760
77:	4	MAIN 770
78:	l'H =',F15.4,1CX,'SFL =',F15.4,2(/),20X,'UST =',F15.4,10X,	MAIN 780
79:	2'UGR =',F15.4,10X,'AM =',F15.4,2(/),2CX,'ANM =',F15.4,10X,	MAIN 790
80:	3'GS =',F15.4,10X,'ALPHA =',F15.4,10X,'AK =',E15.4,2(/),	MAIN PEU
81:	42、X,*X^ =*,E15.4,1^X,*DX =*,E15.4,10X,*RATIC =*,E15.4,1CX,	MAIN 810
82:	52(/),20X,"BETAY =",E15.4,10X,"BETAZ =",E15.4,	MAIN 820
83:	62(/),27X,"D1Y =",E15.4,	MAIN 837
84:	71:X,'D2Y =',E15.4,1UX,'D1Z =',E15.4,17X,'D2Z =',E15.4,2(/),	MAIN 840
85:	820×,*CD1Y =*,E15.4,5×,*DD2Y =*,E15.4,10×,*CD1Z =*,E15.4,5×,	MAIN 857
86:	?*CF2Z =*,E15.4,2(/),2FX,*NY =*,I3,9X,*NZ =*,I3,9X,*ISTB =*,I3,2(/)MAIN 86)
87:	*,20X,"DKN =",F15.4,10X,"DUN =",F15.4,10X,"HSKN =",F15.4,10X,	MAIN 87]
88:	*'HGEO =',F15.4,/)	C88 MIAM
89:	C	NAIN 347
90:	C INITIALIZATION	MAIN SCO
91 :	C	MAIN 910
92:	IUKYP=0	MAIN 920
93:	1 C K Y M = 0	MAIN 93)
94:	I I ()K Y = 0	MAIN 940
95:	IST=J	MAIN 950
95:	FSEL=SEL*F	MAIN 960
97:	DMULY=1.DL	MAIN S7C
93:	DMULZ=1 , DU	MAIN SPC
99:	CICA=CIA	NAIN 990
100:	D1CZ = D1Z	MAINICCO
161:	D2CY=D2Y	MAINICIC
102:	D2^Z=D2Z	MAIN1020
103:	$\nabla T Y = \nabla Y + 2$	MAIN103)
114:	N 1 Y=NY+1	MAIN1040
105:	NTYH=NTY/2	MAIN1051
106:	NTYH1 = NTYH + 1	MAIN1060
1.7:	NTZ = NZ + 2	MAIN1075

			PAGE	4
108:		N 1 Z = N Z + 1	MAIN108	3-0
169:		N P I M=NY*NZ	MAIN109	30
110:	r,		MAIN113	20
111:	С	CALCULATION OF ORTHOGUNAL POINTS, QUADRATURE WEIGHTS,	MAIN111	20
112:	С	AND MATRICES A AND B	MAIN112	20
113:	С		MAIN113	30
114:		CALL JCOBI(12, YY, 1, 1, C. ODO, C. CDC, FAY, FB, FC, RTY)	MAIN114	ŧŪ
115:		CALL CFCPR(12,NY,1,1,I,3,FAY,FR,FC,RTY,WY)	MAIN115	50
116:		UN 457 I=1,NTY	MAIN116	÷C
117:		CALL DFOPR(12, NY, 1, 1, 1, FAY, FB, FC, RTY, VEC)	MAIN117	10
118:		EU = 2 K = 1, NTY	MAIN118	37
119:	2	$2 \Delta Y(I,K) = VEC(K)$	MAIN119	30
120:		CALL DFOPR(12,NY,1,1,I,2,FAY,FB,FC,RTY,VEC)	MA 14120	10
121:		CU = 3 K = 1, NTY	MAIN121	1
12?:	2	BY(I,K)=VEC(K)	MAIN127	> こ
123:	457	CONTINUE	MAIN123	30
124:		CALL JCOBI(12,NZ,1,1,C.ODC,C.CDC,FAZ,FB,FC,RTZ)	MAIN124	+.)
125:		CALL CFCPR(12,NZ,1,1,I,3,FAZ,FB,FC,RTZ,WZ)	MAIN125	51
126:		DC 458 I=1,NTZ	MAIN126	j j
127:		CALL DFOPR(12,NZ,1,1,I,I,FAZ,FB,FC,RTZ,VEC)	MAIN127	17
128:		LG 222 K=1,NTZ	MAIN128	30
129:	222	P AZ(I,K) = VEC(K)	MAIN129	30
130:		CALL DFOPR(12, Z, 1, 1, I, 2, FAZ, FB, FC, RTZ, VFC)	MAIN137	10
131:		CU 333 K=1,NTZ	MAIN131	. J
132:	333	$\exists \exists Z(I,K) = VEC(K)$	MAIN132	2C
133:	458	CONTINUE	MAIN133	n
134:		\\S=NY*NZ	MAIN134	+ O
135:		X = X (MAIN135	50
136:	C		MAIN136	0
137:	С	INITIAL CONDITION DETERMINATION	MAIN137	10
138:	C		MAIN133	31
139:		CALL VELDIF(Z,H,UGP,UST,AM,U,V,ISTB,ALPHA,NTZ,AKYB,AKZB,DAKZB,	MAIN139	; ;
140:		ISEL, C, US, CKN, DUN, HSKN, HGEC, AMM)	MAIN140	20
141:		PV=-UST*DEXP(-SEL*H/AM)*DSIN(SEL*H/AM)/US	MAIN141	. ⁻)
142:		CBX=QS/8.D0/US/YMAX/H/BETAY/BETAZ	MAIN142	20
143:		00 26 J=1+NZ	MAIN143	31

144:		00 26 I=1,NY	MAIN1440
145:		J J = I + (J − 1) * N Y	MAIN1450
146:		PP=1.CD0	MAIN146J
147:		IF((D1Y+D2Y+2.D^*BETAY)*PTY(I+1)-D1Y) 29,28,27	MAIN1475
148:	29	P(JJ)=0.)DC	MAIN148C
149:		CU TO 26	MAIN1490
150:	28	$PP=U \bullet FDO$	MAIN15CO
151:		GO TO 299	MAIN1510
152:	27	IF((D1Y+D2Y+2.DU*BETAY)*RTY(I+1)-D1Y-2.DC*BETAY) 299,298,297	MAIN1520
153:	297	P(JJ)=0.1C0	MAIN153)
154:		GC TC 26	MAIN1540
155:	299	$PP=C \bullet 5DC$	MAIN155C
156:		GU TC 299	MAIN1560
157:	299	IF((D1Z+D2Z+2.D0*BETAZ)*RTZ(J+1)-D1Z) 39,38,37	MAIN1570
159:	39	P(JJ)=J.(DC	MAIN158C
159:		GU TO 26	MAIN1590
16.):	38	P(JJ)=0.5E0*CBX	MAIN1630
161:		6N TO 26	MAIN1610
162:	37	IF((D1Z+D2Z+2.DC*BETAZ)*RTZ(J+1)-D1Z-2.D^*EETAZ) 36,35,34	MAIN1620
163:	34	P(JJ)=0.0E0	MAIN1630
164:		GN TC 26	MAIN1640
165:	35	P(JJ)=^.5DC*CBX	MAIN1650
166:		GU TC 26	MAIN1667
167:	36	P(JJ)=CBX*FP	MAIN1670
168:	26	CONTINUE	DS91NIAM
169:	С		MAIN1690
170:	С	CALCULATION OF EXPRESSIONS USED IN MODEL (DEPENDENT	MAIN17CC
171:	C	OF THE NUMBER OF COLLICATION POINTS ONLY)	MAIN1710
172:	С		MAIN1720
173:		E = NY = AY (NTY, 1) * AY (1, NTY) - AY (1, 1) * AY (NTY, NTY)	MAIN1730
174:		DC 41 I=2,N1Y	MAIN1743
175:		A2Y(I)=AY(1,1)*AY(NTY,I)-AY(NTY,1)*AY(1,I)	MAIN1750
176:		∆1Y(I)=AY(1,I)+AY(1,NTY)*A2Y(I)/DENY	MAIN176)
177:	41	CONTINUE	MAIN1773
178:		DeMZ=AZ(NTZ,1)*AZ(1,NTZ)-AZ(1,1)*AZ(NTZ,NTZ)	MAIN1780
179:		$\Box \cap 441 I=2, N1Z$	MAIN179)

PACE

180:		A 2Z(I)=AZ(1,1)*AZ(NTZ,I)-AZ(NTZ,1)*AZ(1,I)	MAIN1800
181:		A1Z(I)=AZ(1,I)+AZ(1,NTZ)*A2Z(I)/DENZ	MAIN181U
182:	441	CONTINUE	MAIN182C
183:	С		MAIN1830
184:	С	LCOP FUR CHANGING THE BCUNDARY POSITIONS	MAIN1840
185:	С		MAIN1850
186:	50	CONTINUE	MAIN186C
187:		VAR1Y=DABS(D1Y+BETAY-•5DC)	MAIN187C
188:		VAF2Y=DABS(D2Y-1.)D0+.5D0+BETAY)	MAIN1880
189:		VAR1Z=DABS(C1Z+BETAZ-SEL)	MAIN1890
190:		VAR 2Z=DABS(D2Z-1.CDC+SEL+BETAZ)	MAIN1900
191:		WRITE(6,506) D1Y, D2Y, D1Z, D2Z	MAIN1917
192:	56	FCPMAT(5(/),10X,'D1Y =',F10.7,5X,'C2Y =',F10.7,10X,	MAIN1920
193:		1'D12 =',F1C.7,5X,'D22 =',F10.7,1(/))	MAIN1930
194:		DO 8 I=1,NTY	MAIN194)
195:		Y(I)=(D1Y+C2Y+2.D0*BETAY)*RTY(I)+.5C3-BETAY-D1Y	MAIN1950
196:	۶	$ACTY(I) = (2 \cdot DO * Y(I) - 1 \cdot DC) * YMAX$	MAIN1960
197:		CU 888 I=1,NTZ	MAIN1970
193:		Z(I)=(D1Z+C2Z+2.D)*BETAZ)*RTZ(I)+SEL-BETAZ-C1Z	NAIN198C
199:	888	ACTZ(I) = Z(I) * H	MAIN1990
200:		RSEL=(BETAZ+D1Z)/(D1Z+D2Z+2.D0*BETAZ)	MAIN2CUP
201:		PYC=(BETAY+C1Y)/(U1Y+C2Y+2.D^*BETAY)	MAIN2017
202:		ARYC=(2.DC+C.5C ⁻¹ .D ⁰)+YMAX	MAIN2020
203:	С		MAIN2030
204:	С	CALCULATION OF THE DIFFERENTIAL EQUATIONS COEFFICIENTS	MAIN2740
205:	С		MAIN2050
265:		CALL VELDIF(Z,H,UGR,UST,AM,U,V,ISTB,ALPHA,NTZ,AKYE,AKZE,CAKZE,	MAIN2660
207:		1SFL, 1, US, DKN, DUN, HSKN, HGEC, AMM)	MAIN2070
238:		CC 2500 L=2,N1Z	MAIN2080
209:		R1(L)=U(L)/XMAX	MAIN2090
210:		$R_2(L) = V(L)/2 \cdot DL/YMAX/(D1Y+D2Y+2 \cdot DC*BETAY)$	MAIN2100
211:		P3(L) = DAKZE(L)/H/(D1Z+D2Z+2.D)*BETAZ)	MAIN2110
212:		$P5(L) = AKYE(L)/4 \cdot D. /YMAX/YMAX/(C1Y+C2Y+2 \cdot CC*PETAY) * * 2$	MAIN212C
213:		R 6(L) = AKZP(L) /H/H/(D1Z+D2Z+2.DO*BFTAZ)/(D1Z+D2Z+2.CO*BETAZ)	MAIN2130
214:	2000	CCNTINUE	MAIN2141
215:		00 15 K=2,N1Y	MAIN2150

216:	EU 15 I=2,N1Y	MAIN2160
217:	AKY(K,I)=(−BY(K,1)*A1Y(I)/AY(1,1)+BY(K,I)+	MAIN2170
218:	$1 \cup Y(K, NTY) * A2Y(I) / DFNY)$	MAIN2180
219:	AVY(K,I)=(-AY(K,1)*A1Y(I)/AY(1,1)+AY(K,I)+	MAIN2193
22^:	1AY(K,NTY)*A2Y(I)/DENY)	MAIN22CJ
221:	15 CONTINUE	MAIN2210
222:	CU 155 L=2,N1Z	MAIN2220
223:	UC 155 I=2,N1Z	MAIN2230
224:	AKZ(L,I) = (-BZ(L,1) * A1Z(I) / AZ(1,1) + BZ(L,I) +	MAI 12240
225:	1EZ(L, NTZ) * A2Z(I) / DENZ)	MAIN2250
226:	CAKZ(L,I) = (-AZ(L,I) * A1Z(I) / AZ(1,1) + AZ(L,I) +	MAIN226C
227:	$147(L,NTZ) \neq A2Z(I)/DENZ)$	MAIN2270
228:	155 CONTINUE	MAIN2280
229:	CU 10 J=1,NS	MAIN2290
230:	$DC_{IJ}I=1,NS$	MAIN23CC
231:	$I \cap PW(J, I) = C \cdot CD(,$	MA IN2311
232:	CG 113 K=1,NZ	MAIN2327
233:	CC 113 IJ=1,NY	MAIN2330
234:	JJ = IJ + (K-1) * NY	MAIN2340
235:	DO 112 J=1,NZ	NAIN2350
236:	I = I J + (J - 1) * NY	NAIN2360
237:	112 PW(JJ,I)=PW(JJ,I)+AKZ(K+1,J+1)*R6(K+1)/R1(K+1)+	MAIN2373
238:	1EAKZ(K+1,J+1)*R3(K+1)/R1(K+1)	MA IN2380
239:	EU 14 J=1.NY	MAIN2390
247:	I = J + (K - I) * N Y	MAIN2400
241:	14 PW(JJ,I)=PW(JJ,I)+AKY(IJ+1,J+1)*R5(K+1)/R1(K+1)-	MAIN2410
242:	$1 \Delta VY (IJ+1, J+1) * R2(K+1) / R1(K+1)$	MAIN2420
243:	113 CONTINUE	MAIN2430
244:	C	MAIN244C
245:	C INTEGRATION USING DRKGS	NAIN2450
246:	C	MAIN2460
247:	1 CONTINUE	MAIN 2470
248:	$SUM = C \circ DC$	NAIN2480
247:	$KK = N\Gamma IM - 1$	MAIN2491
251:	00 31 I=1.KK	MAIN25C
251:	$\Gamma Y(1) = 1 \cdot D (/ D E CAT(NDIM))$	MAT 12510

			PAGE 8
252:	31	SUM = SUM + DY(I)	MA111252L
253:	_	$CY(NDIM) = 1 \cdot DO - SUM$	NA IN2530
254:		$X^{-}=PRMT(1)$	MAIN2547
255:		D X' = D X	MAIN2550
256:		PRMT(2) = PRMT(1) + DX	MAIN2560
257:		PRMT(3)=CX	MAIN257J
258:		CALL DRKGS(PRMT, P, DY, NCIM, IHLF, FCT, AUX, PW)	MAIN2580
259:		X = PRMT(1)	MAIN259C
260:	65	5 IF(X.GT.1.CCDC) STOP	NAIN2600
261:		IF(X.GE990-07) CX=3.0D-07	MAIN261
262:		IF(X.GE99D-06) DX=3.0D-06	MAIN262C
263:		IF(X.GE99D-05) DX=1.CD-C5	MAIN263C
264:		IF(X.CE99C-04) CX=0.5D-04	MAIN2647
265:		IF(X.GE990-03) DX=0.250-03	MAIN265C
260:		IF(X.GE99D-02) DX=C.25D-(2	MAIN2660
267:		IF(X.GE990-01) LX=0.10D-01	NAIN2677
268:		IF(X.GE499) DX=0.25D-01	MAIN268C
269:		IF(X.GT.C.1D-C1) IICKY=1	MAIN2690
270:	С		MAIN2700
271:	С	TRANSFORMATION OF THE DRKGS RESULTS INTO A C(Y,Z) FORM	MAIN271J
272:	С		MAIN272C
273:		J=1	MAIN2730
274:		L1=1	MAIN2740
275:		L2=NY	MAIN275C
276:	8	L DO 72 L=L1,L2	MAIN276C
277:		K = L - (J - 1) * NY	MAIN2771
278:		K = K + 1	MAIN278C
279:		1 + L = L L	MAIN279C
280:		C(KK, JJ) = P(L)	MAIN2800
281:	7.	CONTINUE	MAIN281C
282:		J = J + 1	MAIN2820
283:		IF(J.GT.NZ) GO TO 82	MAIN2830
284:		L1=L2+1	MAIN2840
285:		L2=L2+NY	MAIN285C
286:		GO TC 81	MAIN286C
287:	53	2 CLNTINUE	MAIN2870

288: C CALCULATION OF THE BOUNDARY CUNCENTRATIONS MAIN2800 289: C CALCULATION OF THE BOUNDARY CUNCENTRATIONS MAIN2800 291: D1 %3 I=1,NTZ MAIN292CC 292: C(1,1)=0.CD0 MAIN2930 293: &3 C(NTY,I)=C.OD0 MAIN2930 294: D0 &33 J=1,NTY MAIN2930 295: C(J,NTZ)=0.CD0 MAIN2950 296: D0 &4 I=2,N1Y MAIN2960 297: D0 &4 I=2,N1Z MAIN2960 297: D0 &4 I=2,N1Z MAIN2960 297: C1,L)=C(I,L)=A1Y(I)*C(I,L)/AY(1,1) MAIN2960 297: D0 &4 I=2,N1Z MAIN2960 297: D0 &4 I=2,N1Z MAIN2960 297: C1,L)=C(I,L)=A1Y(I)*C(I,L)/AY(1,1) MAIN2960 297: C1,L)=C(I,L)=A1Z(I)*C(K,I)/AZ(1,1) MAIN30CC 301: DC &44 H=2,N1Z MAIN3026 302: CU &44 H=2,N1Z MAIN3026 303: C(K,NTZ)=C(K,NTZ)+A2Z(I)*C(I,I)/AY(1,1) MAIN3026 304: C(K,NTZ)+C(I,NTZ)+A2Y(I)*C(I,NTZ)/DENZ MAIN3026 305: C0 &5 I=2,NIY MAIN					
289: C CALCULATION OF THE BOUNDARY CUNCENTRATIONS MAIN2800 291: D() b3 I=1,NTZ MAIN293C 292: C(1,I)=0.CCC MAIN293C 293: B3 C(NTY,1)=C.OD MAIN293C 294: D() 833 J=1,NTY MAIN293C 295: C(J,I)=0.CCC MAIN293C 295: C(J,I)=0.CCC MAIN293C 295: C(J,I)=0.CCC MAIN293C 295: C(J,I)=0.CCC MAIN293C 296: B33 C(J,NTZ]=3.0CO MAIN297D 297: D0 84 L=2,NIZ MAIN297D 293: D0 94 L=2,NIY MAIN297D 294: D0 844 L=2,NIY MAIN297D 301: DC 844 K=2,NIY MAIN297D 302: DU 844 I=2,NIZ MAIN37GC 303: C(K,NT2)=C(K,NT2)+A2Z(I)*C(K,I)/AZ(I,I) MAIN37GC 304: P44 C(K,NT2)=C(K,NT2)+A2Z(I)*C(K,I)/AZ(I,I) MAIN37GC 305: C0 85 I=2,NIY MAIN37GC 306: C1)=C(I,I)=CII,Y)=A2Y(I)*C(I,I)/AY(I,I) MAIN37GC 307: C(I,TY,I)=C(NTY,I)=A2Y(I)*C(I,I)/AY(I,I) MAIN37GC 307: C(I,TY,I)=C(NTY,NTZ)+A2Y(I)*C(I,NTZ)/DENY MAIN37GC 307: C(I,TY,I)=C(NTY,NTZ)+A2Y(I)*C(I,I)/AY(I,I) MAIN37GC 307: C CALCULATICN OF THE EFFCTIVE EMISSICA HEIGHT CONCENTRATION MAIN3	288:	С			MA 142880
291: D1 b2 I=1,NTZ MAIN296C 291: D1 b2 I=1,NTZ MAIN291L 292: C(1,I)=0.CC MAIN2921 293: B3 C(NTY,1)=C.OC MAIN2922 294: D0 033 J=1,NTY MAIN294C 295: C(J,I)=0.CD MAIN294C 296: CJ,I)=0.CD MAIN294C 297: D0 4 L=2,NIZ MAIN297C 293: D0 54 L=2,NIZ MAIN297C 294: C(1,L)=C(I,L)=AIY(I)*C(I,L)/AY(I,I) MAIN297C 297: C(1,L)=C(NTY,L)=AZY(I)*C(I,L)/ZENY MAIN297C 301: DC 844 L=2,NIZ MAIN3CC 302: CU 844 L=2,NIZ MAIN3CC 301: DC 844 L=2,NIZ MAIN3CC 302: CU 844 L=2,NIZ MAIN3CC 304: F44 C(K,NTZ)=C(K,NTZ)+AZZ(I)*C(K,I)/AZ(I,I) MAIN3C5C 305: C0 85 L=2,NIY MAIN3C5C 306: C1,NTZ)=C(I,NTZ)+AZZ(I)*C(I,NTZ)/AY(I,I) MAIN3C5C 306: C0 (I,NTZ)=C(I,NTZ)+AZY(I)*C(I,NTZ)/AY(I,I) MAIN3C5C 307: C (NTY,NTZ)=C(NTY,NTZ)+AZY(I)*C(I,NTZ)/DENY MAIN3C6C 308: <td< td=""><td>289:</td><td>С</td><td></td><td>CALCULATION OF THE BOUNDARY CUNCENTRATIONS</td><td>VAIN2890</td></td<>	289:	С		CALCULATION OF THE BOUNDARY CUNCENTRATIONS	VAIN2890
291: D0 63 1=1,NTZ MAT(291) 292: C(1,T)=0.CC MAIN2920 293: 63 C(NTY,1)=6.*CD MAIN2930 294: D0 333 J=1,NTY MAIN2940 295: C(J,T)=0.CD MAIN2950 296: P33 C(J,NTZ)=3.*CD MAIN2970 297: D0 94 L=2,N1Z MAIN2970 293: D0 94 L=2,N1Y MAIN2970 293: D0 94 L=2,N1Y MAIN2970 293: D0 94 L=2,N1Y MAIN2970 301: DC 44 K=2,N1Y MAIN2970 301: DC 44 K=2,N1Y MAIN3010 302: DU 844 I=2,N1Z MAIN3023 31: C(K,NT2)=C(K,NT2)+A2Y(I)*C(I,L)/A2Y(I,1) MAIN3023 32: DU 844 I=2,N1Y MAIN3024 33: C(K,NT2)=C(K,NT2)+A2Y(I)*C(I,NT2)/A2Y(I,1) MAIN3024 35: D0 85 I=2,N1Y MAIN3024 36: C(I,NT2)=2(I,NT2)-A1Y(I)*C(I,NT2)/A2Y(I,1) MAIN3070 37: C(K,NT2)=C(NTY,NT2)+A2Y(I)*C(I,NT2)/A2Y(I,1) MAIN3070 37: C(I,NT2)=C(I,NT2)-A1Y(I)*C(I,NT2)/A2Y(I,NT2) MAIN3070 37: C(I,NT2)	291:	С			MAIN29CC
292: C(1,1)=0.CCC MAIN2921 293: B3 C(NTY,1)=C.CD MAIN293C 294: D0 B33 J=1,NTY MAIN293C 295: C(J,1)=0.CD MAIN2950 296: P33 C(J,NTZ)=C.OCO MAIN2960 297: D0 P4 L=2,N1Z MAIN2960 293: D0 S4 I=2,N1Y MAIN2960 293: C(1,L)=C(1,L)=AIY(I)*C(I,L)/AY(1,1) MAIN2960 297: C(NTY,L)=C(NTY,L)+A2Y(I)*C(I,L)/DENY MAIN2960 301: DC R44 K=2,N1Z MAIN2960 302: EU 844 I=2,N1Z MAIN2960 301: DC 844 K=2,N1X MAIN30CC 302: EU 844 I=2,N1Z MAIN30C 303: C(K,1)=C(K,NTZ)+A2Z(I)*C(K,I)/AZ(1,1) MAIN30C3 304: EU 844 I=2,N1Z MAIN30C 305: EO 85 I=2,N1Y MAIN30C3 306: C(1,1)=C(I,1)=A1Y(I)*C(I,1)/AY(1,1) MAIN30C3 307: C(I,NTZ)=C(INTY,NTZ)+A2Y(I)*C(I,NTZ)/DENY MAIN30C3 308: C(INTY,NTZ)=C(INTY,NTZ)+A2Y(I)*C(I,NTZ)/DENY MAIN3103 316: C (ALCULATION OF THE EFFFCTIVE CMISSIGN HEIGET CONCENTRATION MAIN3120 <td>291:</td> <td></td> <td></td> <td>DU 63 I=1,NTZ</td> <td>MAIN291U</td>	291:			DU 63 I=1,NTZ	MAIN291U
293: 63 C(NTY,1)=C.ODJ MAIN293C 294: DO 833 J=1,NTY MAIN295C 295: C(J,1)=C.ODJ MAIN295C 296: F33 C(J,NTZ)=0.0EO MAIN295C 297: DO 84 L=2,N1Z MAIN296C 299: C(1,L)=C(1,L)-A1Y(1)*C(1,L)/AY(1,1) MAIN296C 299: C(1,L)=C(1,L)-A1Y(1)*C(1,L)/AY(1,1) MAIN296C 290: C(1,L)=C(1,L)-A1Y(1)*C(1,L)/CENY MAIN296C 301: DC 844 K=2,N1Y MAIN326C 302: CU 844 I=2,N1Z MAIN326C 303: C(K,NTZ)=C(K,NTZ)+A2Z(I)*C(K,I)/AEL,1) MAIN37C 304: P44 C(K,NTZ)=C(K,NTZ)+A2Z(I)*C(K,I)/AEL,1) MAIN37C 305: C0 85 I=2,N1Y MAIN37C 306: C(1,NTZ)=C(1,NTZ)+A2Z(I)*C(I,I)/AEY(1,1) MAIN37C 307: C(K,NTZ)=C(I,NTZ)+A2Z(I)*C(I,NTZ)/AY(1,1) MAIN37C 308: E5 C(NTY,NTZ)=C(NTY,NTZ)+A2Y(I)*C(I,NTZ)/AY(1,1) MAIN3200 316: C MAIN3120 317: CALL UNTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN3120 318: CALL UNTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN3120 319: <t< td=""><td>292:</td><td></td><td></td><td>$C(1, I) = 0 \cdot CDO$</td><td>MAIN292)</td></t<>	292:			$C(1, I) = 0 \cdot CDO$	MAIN292)
294: D0 833 J=1,NTY WAIN2940 295: C(J,1)=0.CDU WAIN2950 296: P33 C(J,NTZ)=2.5CD WAIN2960 297: C0 P4 L=2,N1Z WAIN2970 293: D0 54 I=2,N1Y WAIN2970 293: D0 54 I=2,N1Y WAIN2970 293: D0 54 I=2,N1Y WAIN2970 293: D0 44 I=2,N1Z WAIN2970 301: DC 844 K=2,N1Y WAIN3020 302: CU 844 K=2,N1Z WAIN3720 303: C(K,1)=C(K,NTZ)=42Z(I)*C(K,I)/AZ(I,I) WAIN3720 304: P44 C(K,NTZ)=C(K,NTZ)+A2Z(I)*C(K,I)/AZ(I,I) WAIN3700 305: C0 85 I=2,N1Y WAIN3755 306: C(I,I)=C(I,I)-A1Y(I)*C(I,I)/AY(I,I) WAIN3755 307: C(I,NTZ)=C(NTY,NTZ)-A2Y(I)*C(I,NTZ)/AY(I,I) WAIN3700 307: C(I,NTZ)=C(NTY,NTZ)-A1Y(I)*C(I,NTZ)/DENY WAIN310 308: E5 C(INTY,NTZ)=C(INTY,NTZ)+A2Y(I)*C(I,NTZ)/DENY WAIN310 316: C CALCULATION OF THE EFFFCTIVE EMISSION HEIGHT CONCENTRATION WAIN3120 317: CALL INTRF(12,NTZ,RS*L,RTZ,FAZ,ZINTP) WAIN3120 WAIN3120	293:		۲ 8	C(NTY,I)=CODU	MAIN293C
295: C(J,1)=0.CDU MAIN2950 296: P33 C(J,NTZ)=5.0C0 MAIN2960 297: DD 94 L=2,N1Z MAIN2970 293: DD 94 I=2,N1Y MAIN2970 294: C(I,L)=C(I,L)-AIY(I)*C(I,L)/AY(1,1) MAIN3200 201: DC 844 K=2,N1Y MAIN3207 302: DU 844 I=2,N1Z MAIN3207 303: C(K,I)=C(K,K)I-AIZ(I)*C(K,I)/AZ(1,1) MAIN373 304: F44 C(K,NTZ)=42Z(I)*C(K,I)/AZ(1,1) MAIN370 305: D0 85 I=2,N1Y MAIN370 306: C(I,I)=C(I,I)-AIY(I)*C(I,I)/AY(1,1) MAIN370 307: C(I,NTZ)=C(I,NTZ)-AIY(I)*C(I,NTZ)/AY(1,1) MAIN370 309: E5 C(NTY,NTZ)=C(NTY,NTZ)+A2Y(I)*C(I,NTZ)/AY(1,1) MAIN370 309: E5 C(NTY,NTZ)=C(NTY,NTZ)+RSFL,RTZ,FAZ,ZINTP) MAIN3120 311: C MAIN3120 MAIN3120 312: CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN314C 313: <td< td=""><td>294:</td><td></td><td></td><td>DO 833 J=1,NTY</td><td>MAIN294C</td></td<>	294:			DO 833 J=1,NTY	MAIN294C
296: P33 C(J,NTZ)=0.000 MAIN2960 297: D0 P4 L=2,N1Z MAIN2970 293: D0 S4 I=2,N1Y MAIN2980 299: C(1,L)=C(1,L)-A1Y(I)*C(I,L)/AY(1,1) MAIN2990 301: DC R44 K=2,N1Y 301: DC R44 I=2,N1Y 302: CU 844 I=2,N1Y 303: C(K,I)=C(K,TY,L)+A2Y(I)*C(K,I)/AZ(1,1) MAIN370 304: P44 C(K,NTZ)=C(K,KTZ)+A2Z(I)*C(K,I)/AZ(1,1) MAIN370 305: C0 85 I=2,N1Y MAIN370 306: C(1,I)=C(1,I)-A1Y(I)*C(K,I)/AZ(1,1) MAIN370 MAIN370 307: C(1,I)=C(I,T)-A1Y(I)*C(K,I)/AY(1,1) MAIN360 MAIN360 309: E5 C(NTY,NTZ)=C(NTY,NTZ)-A1Y(I)*C(I,NTZ)/AY(1,1) MAIN3100 309: E5 C(NTY,NTZ)=C(NTY,NTZ)-A2Y(I)*C(I,NTZ)/AY(1,1) MAIN3200 310: CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN3110 311: CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN3120 313: CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN3120	295:			$C(J, 1) = 0 \cdot CDU$	MAIN2950
297: D0 94 L=2,N1Z MAIN2970 293: D0 94 I=2,N1Y MAIN2980 299: C(1,L)=C(1,L)-A1Y(1)*C(1,L)/A2Y(1,1) MAIN2990 307: B4 C(NTY,L)=C(NTY,L)+A2Y(I)*C(I,L)/CENY MAIN3290 301: DC 844 K=2,N1Y MAIN320 301: DC 844 K=2,N1Z MAIN320 302: C(K,1)=C(K,NTZ)+A2Z(I)*C(K,I)/AZ(1,1) MAIN370 302: C(K,1)=C(K,NTZ)+A2Z(I)*C(K,I)/CENZ MAIN3750 304: P44 C(K,NTZ)=C(K,NTZ)+A2Z(I)*C(I,1)/CENZ MAIN3760 305: D0 85 I=2,N1Y MAIN3750 306: C(1,1)=C(I,1)-A1Y(I)*C(I,1)/CENY MAIN3760 307: C(NTY,I)=C(NTY,I)+A2Y(I)*C(I,NTZ)/AY(I,1) MAIN3700 308: C(I,NTZ)=C(INTZ)-A1Y(I)*C(I,NTZ)/DENY MAIN3700 310: CALL INTRF(12,NTZ)-RSFL,RTZ,FAZ,ZINTP) MAIN3120 313: CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN3120 314: D0 855 J=1,NTY MAIN3160 315: EHCO(J)=0.0G MAIN3160 316: C MAIN3160 317: F55 EHCO(J)=EHCC(J)+ZINTP(I)*C(J,I) MAIN3160 317: <	296:		833	C(J, NTZ) = 0.0D0	MAIN2960
293: D0 94 I=2,NIY MAIN2980 297: C11,L)=C(11,L)-A1Y(I)*C(I,L)/AY(1,1) MAIN2990 297: C(NTY,L)=C(NTY,L)+A2Y(I)*C(I,L)/CENY MAIN2900 301: DC 844 K=2,NIY MAIN3010 302: CU 844 I=2,NIZ MAIN3020 313: C(K,I)=C(K,NTZ)+A2Z(I)*C(K,I)/AZ(1,1) MAIN30302 324: P44 C(K,NTZ)=C(K,NTZ)+A2Z(I)*C(K,I)/AENZ MAIN30302 305: D0 85 I=2,NIY MAIN30302 306: C(I,I)=C(I,I)-A1Y(I)*C(I,I)/AY(I,I) MAIN30303 307: C5 I=2,NIY MAIN30303 308: C(I,NTZ)=C(I,NTZ)-A1Y(I)*C(I,I)/AY(I,I) MAIN30303 309: E5 C(NTY,NTZ)=C(NTY,NTZ)+A2Y(I)*C(I,NTZ)/AY(1,I) MAIN30303 309: E5 C(NTY,NTZ)=C(NTY,NTZ)+A2Y(I)*C(I,NTZ)/DENY MAIN3100 310: CALLUATION OF THE EFFECTIVE CMISSION HEIGHT CONCENTRATION MAIN3120 313: CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN3120 314: D0 855 J=1,NTZ MAIN3120 315: EHCO(J)=0,DG MAIN3160 316: C MAIN3160 317: P55 LHCO(J)=EFECC(J)+ZINTP(I)*C(J,I) MAIN3160	297:			DO 84 L=2,N1Z	MAIN2970
299: C(1,L)=C(1,L)-A1Y(1)*C(1,L)/AY(1,1) MAIN3207 301: DC 844 K=2,N1Y MAIN3C1 302: DC 844 K=2,N1Y MAIN3C1 302: DC 844 K=2,N1Y MAIN3C2 303: C(K,1)=C(K,NTZ)+A2Y(I)*C(K,I)/AZ(1,1) MAIN3C23 31: C(K,1)=C(K,NTZ)+A2Z(I)*C(K,I)/AZ(1,1) MAIN3C3C 324: 844 C(K,NTZ)=C(K,NTZ)+A2Z(I)*C(K,I)/AENZ MAIN3C60 35: C0 85 I=2,N1Y MAIN3C50 36: C(1,1)=C(1,1)-A1Y(I)*C(I,1)/AY(1,1) MAIN3C50 37: C(INTY,I)=C(INTY,I)+A2Y(I)*C(I,NTZ)/AY(1,1) MAIN3C60 37: C(INTY,I)=C(INTY,I)+A2Y(I)*C(I,NTZ)/AY(1,1) MAIN3C60 37: C(INTY,I)=C(INTY,I)+A2Y(I)*C(I,NTZ)/AY(1,1) MAIN3C60 37: C(INTY,I)=C(INTY,I)+A2Y(I)*C(I,INTZ)/DENY MAIN3C60 37: C(INTY,ITZ)=C(INTY,ITZ)+A2Y(I)*C(I,INTZ)/DENY MAIN3C60 37: CALCULATION OF THE EFFECTIVE EMISSION HEIGHT CONCENTRATION MAIN3120 314: NO 855 J=1,NTY MAIN3120 MAIN3120 314: NO 855 J=1,NTZ MAIN3160 MAIN3160 317: CALCULATION OF THE CONCENTRATIONS AT Y=0 MAIN3180 <	293:			DO 84 I = 2.N1Y	MAIN2980
301: 84 C(NTY,L)=C(NTY,L)+A2Y(I)*C(I,L)/CENY MAIN3CC 301: DC 844 K=2,N1Y MAIN3C10 302: C(K,I)=C(K,I)-A1Z(I)*C(K,I)/AZ(1,I) MAIN3C3C 3'3: C(K,I)=C(K,NTZ)=C(K,NTZ)+A2Z(I)*C(K,I)/AZ(1,I) MAIN3C3C 3'4: P44 C(K,NTZ)=C(K,NTZ)+A2Z(I)*C(K,I)/AZ(1,I) MAIN3C4C 3'5: C0 85 I=2,N1Y MAIN3C4C 3'6: C(I,I)=C(I,I)-A1Y(I)*C(I,I)/AY(1,I) MAIN3C6C 3'7: C(I,NTZ)=C(I,NTZ)-A1Y(I)*C(I,NTZ)/AY(1,I) MAIN3C80 3'9: &F C(NTY,NTZ)=C(NTY,NTZ)+A2Y(I)*C(I,NTZ)/DENY MAIN3C80 3'9: &F C(NTY,NTZ)=C(NTY,NTZ)+A2Y(I)*C(I,NTZ)/DENY MAIN3C80 3'1: CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN3120 3'13: CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN3120 3'14: D0 855 J=1,NTZ MAIN3160 3'14: D0 855 J=1,NTZ MAIN3160 3'17: F55 LHC0(J)=EHCC(J)+ZINTP(I)*C(J,I) MAIN3170 3'18: C MAIN3160 3'19: CALCULATICN OF THE CONCENTRATIONS AT Y=0 MAIN3180 3'19: CALCULATICN OF THE CONCENTRATIONS AT Y=0 MAIN3190 3'19:	299:			C(1,L) = C(1,L) - A1Y(1) * C(1,L) / AY(1,1)	MAIN2990
301: DC 844 K=2,NIY VAIN3010 302: DU 844 I=2,NIZ MAIN3020 3'3: C(K,I)=C(K,I)-AIZ(I)*C(K,I)/AZ(I,I) MAIN3020 3'4: P44 C(K,NTZ)=C(K,NTZ)+A2Z(I)*C(K,I)/CENZ MAIN3050 3'5: D0 85 I=2,NIY MAIN3050 3'6: C(I,I)=C(I,I)-AIY(I)*C(I,I)/AY(I,I) MAIN3050 3'7: C(NTY,I)=C(NTY,I)+A2Y(I)*C(I,I)/AY(I,I) MAIN3070 3'7: C(I,NTZ)=CI(NTZ)-AIY(I)*C(I,NTZ)/AY(I,I) MAIN3070 3'7: C(I,NTZ)=C(I,TZ)-AIY(I)*C(I,NTZ)/DENY MAIN3070 3'7: CALCULATION OF THE EFFFCTIVE DMISSION HEIGHT CONCENTRATION MAIN3120 3'11: C CALCULATION OF THE EFFFCTIVE DMISSION HEIGHT CONCENTRATION MAIN3120 3'13: CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN3120 MAIN3120 3'14: NO 855 J=1,NTZ MAIN3140 MAIN3140 3'16: C 00 855 J=1,NTZ MAIN3120 MAIN3120 3'17: F55 EHCO(J)=EHCC(J)+ZINTP(I)*C(J,I) MAIN3120 MAIN3120 3'18: C CALCULATION OF THE CONCENTRATIONS AT Y=0 MAIN3120 3'17: CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP) MAIN3200	301:		84	C(NTY,L)=C(NTY,L)+A2Y(I)*C(I,L)/CENY	MAINBCCC
302: CU 844 I=2,NIZ MAIN3^20 3'3: C(K,1)=C(K,1)-A1Z(I)*C(K,I)/AZ(1,1) MAIN3^3C 324: P44 C(K,NTZ)=C(K,NTZ)+A2Z(I)*C(K,I)/DENZ MAIN3^3C 305: C0 85 I=2,NIY MAIN3^50 3'6: C(1,1)=C(1,1)-A1Y(I)*C(I,1)/AY(1,1) MAIN3^50 3'7: C(NTY,1)=C(NTY,1)+A2Y(I)*C(I,1)/CENY MAIN3070 308: C(1,NTZ)=C(1,NTZ)-A1Y(I)*C(I,NTZ)/AY(1,1) MAIN3080 310: CALCULATION OF THE EFFECTIVE EMISSION HEIGHT CONCENTRATION MAIN3120 311: C CALCULATION OF THE EFFECTIVE EMISSION HEIGHT CONCENTRATION MAIN3120 312: C MAIN3120 MAIN3120 313: CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN3120 314: D0 855 J=1,NTZ MAIN314C MAIN3150 316: C0 855 I=1,NTZ MAIN3160 MAIN3170 316: C0 855 I=1,NTZ MAIN3170 MAIN3170 316: C MAIN3170 MAIN3180 317: F55 EHCO(J)=EHCC(J)+ZINTP(I)*C(J,I) MAIN3170 MAIN3170 318: C MAIN3200 MAIN3180 MAIN3200 321:	301:			DC 844 K=2,N1Y	MAIN3010
3'3: C(K,1)=C(K,1)-AIZ(I)*C(K,I)/AZ(1,1) MAIN3C3C 3C4: 844 C(K,NTZ)=C(K,NTZ)+A2Z(I)*C(K,I)/CENZ MAIN3C4C 3D5: CD 85 I=2,NIY MAIN3C4C 3C6: C(1,1)=C(1,1)-A1Y(I)*C(I,1)/AY(1,1) MAIN3C6C 3C7: C(1,NTZ)=C(NTY,1)+A2Y(I)*C(I,1)/AY(1,1) MAIN3C8O 3C8: C(1,NTZ)=C(NTY,NTZ)+A2Y(I)*C(I,NTZ)/AY(1,1) MAIN3C8O 3C9: & 5 C(NTY,NTZ)=C(NTY,NTZ)+A2Y(I)*C(I,NTZ)/DENY MAIN3C8O 310: C CALCULATION OF THE EFFFCTIVE CMISSION HEIGHT CONCENTRATION MAIN312D 311: C CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN312D 314: DU 855 J=1,NTY MAIN312D 315: EHCO(J)=0.DG MAIN314C MAIN316D 316: C MAIN316D MAIN316D 316: EHCO(J)=EHCC(J)+ZINTP(I)*C(J,I) MAIN316D MAIN316D 317: F55 EHCO(J)=EHCC(J)+ZINTP(I)*C(J,I) MAIN316D MAIN316D 318: C MAIN318D MAIN318D MAIN312D 317: F55 EHCO(J)=EHCC(J)+ZINTP(I)*C(J,I) MAIN318D MAIN312D	302:			EU 844 I = 2.N1Z	MAIN3020
324: 844 C(K,NTZ)=C(K,NTZ)+A2Z(I)*C(K,I)/CENZ MAIN3040 305: C0 85 I=2,NIY MAIN3050 36: C(I,I)=C(I,I)-A1Y(I)*C(I,I)/AY(I,I) MAIN3050 36: C(I,I)=C(I,I)-A1Y(I)*C(I,I)/CENY MAIN3070 308: C(I,NTZ)=C(I,NTZ)-A1Y(I)*C(I,NTZ)/AY(I,I) MAIN3070 309: 85 C(NTY,NTZ)=C(NTY,I)+A2Y(I)*C(I,NTZ)/AY(I,I) MAIN3070 309: 85 C(NTY,NTZ)=C(NTY,I)+A2Y(I)*C(I,NTZ)/DENY MAIN3070 316: C MAIN3120 311: C CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN3120 313: CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN3120 314: D0 855 J=1,NTY MAIN3140 MAIN3140 315: EHCO(J)=0.00 MAIN3160 MAIN3160 316: C0 855 I=1,NTZ MAIN3160 MAIN3160 316: C0 855 I=1,NTZ MAIN3180 MAIN3180 316: C MAIN3120 MAIN3180 MAIN3120 316: C MAIN3120 MAIN3180 MAIN3120 317: F55 EHCO(J)=EHCC(J)+ZINTP(I)*C(J,I) MAIN3120 MAIN3120	3 '3:			C(K,1) = C(K,1) - A1Z(I) * C(K,I) / AZ(1,1)	MAIN 303C
335: D0 85 I=2,NIY MAIN3050 3^6: C(1,1)=C(1,1)-AIY(I)*C(I,1)/AY(1,1) MAIN3070 36: C(NTY,1)=C(NTY,1)+A2Y(I)*C(I,NTZ)/AY(1,1) MAIN3070 308: C(I,NTZ)=C(I,NTZ)-AIY(I)*C(I,NTZ)/AY(1,1) MAIN3070 309: 85 C(NTY,NTZ)=C(INTY,I)*A2Y(I)*C(I,NTZ)/DENY MAIN3090 316: C MAIN3120 311: C CALCULATION OF THE EFFECTIVE DMISSION HEIGHT CONCENTRATION MAIN3120 312: C MAIN3120 MAIN3120 313: CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN3130 MAIN3140 314: D0 855 J=1,NTY MAIN3150 MAIN3160 315: EHCO(J)=0.DG MAIN3160 MAIN3160 316: C0 855 I=1,NTZ MAIN3160 MAIN3180 317: 855 EHCO(J)=EFCC(J)+ZINTP(I)*C(J,I) MAIN3180 MAIN3180 319: C CALCULATION OF THE CONCENTRATIONS AT Y=0 MAIN3190 321: CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP) MAIN3220 MAIN3220 322: CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP) MAIN3220 MAIN3220 322: CALL INTRP(12,NTZ,RYC,RTY,FAY,YIN	334:		844	C(K,NTZ) = C(K,NTZ) + A2Z(I) * C(K,I)/CENZ	MAIN 3040
3^6: C(1,1)=C(1,1)-A1Y(I)*C(I,1)/AY(1,1) MAIN3C6C 3C7: C(NTY,1)=C(NTY,1)+A2Y(I)*C(I,1)/DENY MAIN3070 308: C(1,NTZ)=C(1,NTZ)-A1Y(I)*C(I,NTZ)/AY(1,1) MAIN3070 309: 85 C(NTY,NTZ)=C(NTY,NTZ)+A2Y(I)*C(I,NTZ)/DENY MAIN3070 316: C MAIN3070 MAIN3070 316: C CALCULATION OF THE EFFECTIVE DMISSION HEIGHT CONCENTRATION MAIN3120 313: CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN3120 314: D0 855 J=1,NTY MAIN3120 314: D0 855 J=1,NTY MAIN314C 315: EHCO(J)=0.06 MAIN3150 316: C 0 855 I=1,NTZ MAIN3160 317: F55 EHCO(J)=EHCC(J)+ZINTP(I)*C(J,I) MAIN3160 318: C MAIN3160 317: F55 EHCO(J)=EHCC(J)+ZINTP(I)*C(J,I) MAIN3180 318: C MAIN3180 319: C MAIN3180 320: CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP) MAIN3200 321: CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP) MAIN3210 322: CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP) MAIN3200 <td>305:</td> <td></td> <td></td> <td>CO 85 I=2.N1Y</td> <td>MAIN3050</td>	305:			CO 85 I=2.N1Y	MAIN3050
3C7: C(NTY,1)=C(NTY,1)+A2Y(I)*C(I,1)/DENY MAIN3070 3C8: C(1,NTZ)=C(1,NTZ)-A1Y(I)*C(I,NTZ)/AY(1,1) MAIN3070 3C9: &5 C(NTY,NTZ)=C(NTY,NTZ)+A2Y(I)*C(I,NTZ)/DENY MAIN3070 316: C MAIN3070 MAIN3070 316: C MAIN3070 MAIN3070 311: C CALCULATION OF THE EFFECTIVE EMISSION HEIGHT CONCENTRATION MAIN3110 312: C MAIN3120 MAIN3120 313: CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN3120 314: D0 855 J=1,NTY MAIN3120 315: EHCO(J)=0.D0 MAIN3150 316: EO 855 I=1,NTZ MAIN3160 317: F55 EHCO(J)=EHCC(J)+ZINTP(I)*C(J,I) MAIN3170 318: C MAIN3180 319: C CALCULATION OF THE CONCENTRATIONS AT Y=0 MAIN3190 321: CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP) MAIN3200 322: ED 856 J=1,NTZ MAIN320 322: ED 856 J=1,NTZ MAIN320	3^6:			C(1,1) = C(1,1) - A1Y(1) * C(1,1) / AY(1,1)	MAIN3C6C
308: C(I,NTZ)=C(I,NTZ)-AlY(I)*C(I,NTZ)/AY(I,1) MAIN3090 309: 85 C(NTY,NTZ)=C(NTY,NTZ)+A2Y(I)*C(I,NTZ)/DENY MAIN3090 316: C MAIN3090 MAIN3090 316: C MAIN3090 MAIN3090 311: C CALCULATION OF THE EFFECTIVE DMISSION HEIGHT CONCENTRATION MAIN3110 312: C MAIN3120 MAIN3120 313: CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN3130 314: NO 855 J=1,NTY MAIN3140 315: EHCO(J)=0.D6 MAIN3150 C0 855 I=1,NTZ MAIN3160 MAIN3170 316: C0 855 I=1,NTZ MAIN3170 317: P55 EHCO(J)=EFCC(J)+ZINTP(I)*C(J,I) MAIN3170 318: C MAIN3180 319: C CALCULATION OF THE CONCENTRATIONS AT Y=0 MAIN3190 320: CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP) MAIN3220 MAIN3220 321: CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP) MAIN3220 MAIN3220 322: C0 856 J=1,NTZ MAIN3220 MAIN3220	367:			C(NTY,1) = C(NTY,1) + A2Y(I) * C(I,1) / CENY	MAIN 3070
309: &F C(NTY,NTZ)=C(NTY,NTZ)+A2Y(I)*C(I,NTZ)/DENY MAIN3090 316: C MAIN3090 311: C CALCULATION OF THE EFFECTIVE DRISSION HEIGHT CONCENTRATION MAIN3110 312: C MAIN3120 MAIN3120 313: CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN3130 314: D0 855 J=1,NTY MAIN3140 315: EHCO(J)=0.06 MAIN3150 316: EHCO(J)=0.06 MAIN3150 317: F55 EHCO(J)=EHCC(J)+ZINTP(I)*C(J,I) MAIN3170 318: C C 319: C CALCULATION OF THE CONCENTRATIONS AT Y=0 327: C MAIN3190 321: CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP) MAIN3200 322: COMENTRATIONS AT Y=0 MAIN3220 321: CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP) MAIN3220 322: COMENTRATION FOR THE CONCENTRATIONS AT Y=0 MAIN3220	308:			C(1, NTZ) = C(1, NTZ) - A1Y(1) * C(1, NTZ) / AY(1, 1)	MAIN3C80
316:CMAIN31CC311:CCALCULATION OF THE EFFECTIVE EMISSION HEIGHT CONCENTRATIONMAIN3110312:CMAIN3120313:CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP)MAIN3120314:D0 855 J=1,NTYMAIN3130315:EHCO(J)=0.D0MAIN3140316:EHCO(J)=0.D0MAIN3150316:EHCO(J)=EHCC(J)+ZINTP(I)*C(J,I)MAIN3160317:P55 EHCO(J)=EHCC(J)+ZINTP(I)*C(J,I)MAIN3180318:CMAIN3180319:CCALCULATION OF THE CONCENTRATIONS AT Y=0MAIN3190324:CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP)MAIN3210322:E0 856 J=1,NTZMAIN3220322:CO 856 J=1,NTZMAIN3220323:COCCHU STMAIN3220324:CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP)MAIN3220325:CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP)MAIN3220326:CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP)MAIN3220327:CMAIN3220328:COCCHU ST	309:		85	C(NTY, NTZ) = C(NTY, NTZ) + A2Y(I) * C(I, NTZ) / DENY	MAIN3790
311:CCALCULATION OF THE EFFECTIVE EMISSION HEIGHT CONCENTRATIONMAIN3115312:CMAIN3120MAIN3120313:CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP)MAIN313C314:D0 855 J=1,NTYMAIN314C315:EHCO(J)=0.DGMAIN3150316:CO 855 I=1,NTZMAIN3160317:F55 EHCO(J)=EHCC(J)+ZINTP(I)*C(J,I)MAIN317C318:CCALCULATION OF THE CONCENTRATIONS AT Y=0MAIN3190327:CCALL INTRP(12,NTY,RYC,RTY,FAY,YINTP)MAIN3210322:CO 856 J=1,NTZMAIN3220322:CO 856 J=1,NTZMAIN3220	310:	С			MAIN21CC
312: C MAIN312D 313: CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN313C 314: DD 855 J=1,NTY MAIN314C 315: EHCO(J)=0.DG MAIN315D 316: ED 855 I=1,NTZ MAIN316D 317: P55 EHCD(J)=EHCC(J)+ZINTP(I)*C(J,I) MAIN316D 318: C MAIN318D 319: C CALCULATION OF THE CONCENTRATIONS AT Y=C MAIN319D 320: C CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP) MAIN322D 322: ED 856 J=1,NTZ MAIN322D 322: ED 856 J=1,NTZ MAIN322D	311:	č		CALCULATION OF THE EFFECTIVE EMISSION HEIGHT CONCENTRATION	MAIN3115
313: CALL INTRF(12,NTZ,RSFL,RTZ,FAZ,ZINTP) MAIN313C 314: D0 855 J=1,NTY MAIN314C 315: EHCO(J)=0.DG MAIN3150 316: CO 855 I=1,NTZ MAIN3160 317: F55 EHCO(J)=EHCC(J)+ZINTP(I)*C(J,I) MAIN317C 318: C MAIN3180 319: C CALCULATION OF THE CONCENTRATIONS AT Y=0 MAIN3190 327: C MAIN320C MAIN3210 322: CO 856 J=1,NTZ MAIN3210 MAIN3220 322: CO 856 J=1,NTZ MAIN3220 MAIN3220	312:	Č			MAIN3120
314: D0 855 J=1,NTY MAIN314C 315: EHCO(J)=0.DG MAIN3150 316: EO 855 I=1,NTZ MAIN3160 317: F55 EHCO(J)=EHCC(J)+ZINTP(I)*C(J,I) MAIN3170 318: C MAIN3180 319: C CALCULATION OF THE CONCENTRATIONS AT Y=0 MAIN3180 327: C MAIN3200 MAIN3210 321: CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP) MAIN3210 322: EO 856 J=1,NTZ MAIN3220	313:	•		CALL INTRE(12.NT7.RSEL.RT7.EA7.7INTP)	MAINBIBC
315: EHCO(J)=0.DG 316: EO 855 I=1.NTZ 317: F55 EHCO(J)=EHCC(J)+ZINTP(I)*C(J,I) 318: C 319: C CALCULATION OF THE CONCENTRATIONS AT Y=C MAIN3190 327: C 321: CALL INTRP(12.NTY,RYC.RTY,FAY,YINTP) 322: EO 856 J=1.NTZ 322: CO 856 J=1.NTZ 322: CO 856 J=1.NTZ	314:			DO 855 J=1.NTY	MAINBIAC
316: EO 855 I=1,NTZ 317: F55 EHCO(J)=EHCC(J)+ZINTP(I)*C(J,I) 318: C 319: C CALCULATION OF THE CONCENTRATIONS AT Y=C MAIN3190 327: C 321: CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP) 322: EO 856 J=1,NTZ 323: C550(1)=105	315:			EHCD(J)=0.DC	NAIN3150
317: F55_EHCO(J)=EHCC(J)+ZINTP(I)*C(J,I) 318: C 319: C CALCULATION OF THE CONCENTRATIONS AT Y=C MAIN3190 327: C 321: CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP) 322: CO 856 J=1,NTZ MAIN3220 MAIN3220	316:			$\Gamma_{0} = 855 I = 1 \cdot NT7$	NAIN3160
318:C319:CCCALCULATION OF THE CONCENTRATIONS AT Y=CMAIN3190320:C321:CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP)322:D0 856 J=1,NTZ322:C500(1)=1,NTZ322:C500(1)=1,NTZ	317:		ទភ្ន	E H C D (J) = E E C C (J) + 7 I N T P (J) * C (J, J)	MAINBITC
319: CCALCULATION OF THE CONCENTRATIONS AT Y=CMAIN3190320: CMAIN32CCMAIN32CC321: CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP)MAIN3210322: C0 856 J=1,NTZMAIN3220323: C550(1)=0.55MAIN3220	318:	С	-		NAIN3180
327: C MAIN32CC 321: CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP) MAIN3210 322: CO 856 J=1,NTZ MAIN3220 323: CO 856 J=1,NTZ MAIN3220	319:	č		CALCULATION OF THE CONCENTRATIONS AT $Y=0$	MAIN3190
321: CALL INTRP(12,NTY,RYC,RTY,FAY,YINTP) MAIN3210 322: DD 856 J=1,NTZ MAIN3220 323: C550(1)=0.55 MAIN3230	320:	ć			MAINB2CC
322: DO 856 J=1,NTZ MAIN3220	321:	~		CALL INTRP(12.NTY.RYC.RTY.FAY.YINTP)	MATN 3210
	322:			$\Gamma \Omega = 856 \ J=1 \cdot NT7$	MATN3221
DYDE UFUUUUEDEN MAINEZ MAL	323:			$CECC(J) = 0 \cdot CC$	MAIN323C

324: CD 856 1=1,NTY MA1N3245 325: F56 C_CO(J)=CECC(J)+YINTP(I)*C(I,J) MA1N3255 326: CCO1=C.DC MAIN3265 327: CCU2=n.CD MAIN3267 328: CCCC3=n.D.J MAIN3267 329: DO 957 I=1,NTY MAIN3267 329: CC01=CC01+YINTP(I)*EHCO(I) MAIN3267 331: 657 CONTINUF MAIN3212 332: C(Y=EHCO(I) MAIN3321 332: CIY=FHCO(INTY) MAIN3321 333: C MAIN3333 334: C MAIN3363 335: C CALCLLATICN CF THE MASS RATE MAIN3363 336: D 47 I=2,NIY MAIN3363 337: D0 47 I=2,NIY MAIN3363 MAIN3363 340: G AAIN3343 MAIN3363 341: G=2+CNYMMAX+(CIY+CZ+2+C)*BETAY)*H*(DIZ+CZ+2+CU*BETAZ)*C MAIN3463 342: D=1CC,C,DC/CC MAIN34343 MAIN34343 344: C AATX=XMAX MAIN34343 345: C CALCLLATICN CF THE TRUE CENTERLINE CCNCENTRATIONS					
325: 6.56 C_CO(J)=CECC(J)+YINTP(I)*C(I,J) MAIN3250 326: CCO1=C+OC MAIN3260 327: CCU2=0.00 MAIN3270 328: CCO3=0.00 MAIN3270 328: CCO3=0.00 MAIN3270 329: DO 857 I=1.NTY MAIN3290 331: 657 CONTINUF MAIN32300 332: CIY=EHCO(I) MAIN32300 333: CIY=EHCO(I) MAIN33300 334: C MAIN32300 335: C CALCULATICN CF THE MASS RATE MAIN3360 336: C MAIN3250 MAIN3250 337: C=0.*C*0 MAIN3370 MAIN3370 338: D0 47 I=2.NIY MAIN3250 MAIN3250 341: C=2.0*WMAX*(CIY+C2Y+2.0*C#HETAY)*H*(DIZ+CZ7+2.0*C#BETAZ)*C MAIN3400 341: C=2.0*WMAX*(CIY+C2Y+2.0*C#HETAY)*H*(DIZ+CZ7+2.0*C#BETAZ)*C MAIN3420 342: Q=10*C,0*C*0*C*0 MAIN3420 MAIN3433 343: C MAIN3450 MAIN3450 344: C MAIN3450 MAIN3450 345: C ALCULATICN CF THE TRUE	324:			ED 856 I=1,NTY	MAIN3240
326: CC(1)=C+0C MAIN3262 327: CC(2)=0C MAIN3273 328: CCC3=0.0 MAIN3282 329: DO 857 I=1,NTY MAIN3282 327: CC01=C001+YINTP(1)*EHCO(I) MAIN3283 331: 657 CONTINUE MAIN3333 332: C1Y=EHCO(NTY) MAIN3333 334: C MAIN3353 335: C CALCULATICN CF THE MASS RATE MAIN3353 336: DO 47 I=2,NIY MAIN3363 337: C=0+CO MAIN3363 338: DO 47 I=2,NIY MAIN3363 339: DO 47 I=2,NIY MAIN3363 341: C=2+CO+WMX+(C1Y+D2Y+2+DO+HETAY)*H*(D1Z+C27+2+UC*BETAZ)*C MAIN3403 341: C=2+CO+WMX+(C1Y+D2Y+2+DO+HETAY)*H*(D1Z+C27+2+UC*BETAZ)*C MAIN3420 342: O=1CC+0C/6C+0C+VC MAIN3420 MAIN3420 344: C MAIN3420 MAIN3420 344: C MAIN3420 MAIN3420 344: C MAIN3420 MAIN3420 347: RYC=(RETAY+C1Y+PV*ACTX/2+CC/YMAX)/(D1Y+D2Y+2+D0*BETAY) MAIN3420 <	325:		826	C = CO(J) = CECC(J) + YINTP(I) * C(I, J)	MAIN325C
327: CCU2=n.CO MAIN3273 328: CCO3=n.DJ MAIN3273 329: DD 957 I=1,NTY MAIN3262 337: CCU1=CCU1+INTP(I)*EHCU(I) MAIN3307 331: 657 CONTINUE MAIN3327 332: C1Y=EHCU(1) MAIN3312 332: C1Y=EHCU(1) MAIN3333 334: C MAIN3347 335: C CALCULATION OF THE MASS RATE MAIN3350 336: C MAIN3353 337: C=0.000 MAIN3350 338: DU 47 I=2.NIY MAIN3360 340: 47 C=0.4NIX MAIN3400 341: C=2.0019/MAX(014002)+E2.000*BETAZ)*C MAIN3420 342: D=100/CC.00/ACC.00*C MAIN3420 343: ACTX=XXMAX MAIN3420 344: C MAIN3420 344: C MAIN3420 344: C	326:			CCOl=C.DC	MAIN3260
323: CC03=0.0.J MAIN32PC 329: DD 957 I=1,NTY MAIN32PC 331: 657 CONTINUE MAIN3312 332: C(Y=EHCO(1) MAIN332C 333: C1Y=EHCO(NTY) MAIN33312 334: C MAIN332C 335: C1Y=EHCO(INTY) MAIN3333 336: C MAIN3363 337: C=0.000 MAIN3363 338: D0 47 J=2,NIY MAIN3363 339: D0 47 J=2,NIY MAIN3363 341: C=0.000 MAIN3363 342: 0=100.700 MAIN3403 341: C=0.100.700 MAIN3403 342: 0=100.700.700 MAIN3403 344: C MAIN3420 344: C MAIN3423 344: C MAIN3423 347: RYC=(RETAY+CIY+PV*ACTX/2.0C/YMAX)/(DIY+D2Y+2.00*BETAY) MAIN3426 344: C MAIN3426 MAIN3426 347: RYC=(RETAY+CIY+PV*ACTX/2.0C/YMAX)/(DIY+D2Y+2.00*BETAY) MAIN3426 357: CLQLLATICN CF THE TRUE CENTERLINE CONCENTRATICNS </td <td>327:</td> <td></td> <td></td> <td>CCU2=0.00</td> <td>MAIN3270</td>	327:			CCU2=0.00	MAIN3270
329: DD 957 I=1,NTY MAIN3290 331: 657 CONTINUF MAIN3312 332: C1Y=EHCO(1) MAIN3320 333: C1Y=EHCO(NTY) MAIN3340 336: C MAIN3360 337: C=0.000 MAIN3370 338: D0 47 I=2,N12 MAIN3370 338: D0 47 I=2,N12 MAIN3360 339: C0 47 J=2,N12 MAIN3360 341: C=2.004YMAX*(C1Y+C2Y+2.00*BETAY)*H*(D12+C27+2.00*BETAZ)*C MAIN3400 341: C=2.004YMAX*(C1Y+C2Y+2.00*BETAY)*H*(D12+C27+2.00*BETAZ)*C MAIN3400 341: C=2.004YMAX*(C1Y+C2Y+2.00*BETAY)*H*(D12+C27+2.00*BETAZ)*C MAIN3400 341: C=2.004YMAX*(C1Y+C2Y+2.00*BETAY)*H*(D12+C27+2.00*BETAZ)*C MAIN3400 342: O=1000,C00.00*C MAIN3430 344: C MAIN3400 347: RYC=(RETAY+C1Y+PV*ACTX/2.000/YMAX)/(D1Y+D2Y+2.006*BETAY) <	328:			CC03=0.DJ	MAIN3280
33C: CC01=CC01+YINTP(I)*EHC0(I) MAIN33C; 331: 657 CGNTINUF MAIN33C; 331: 657 CGNTINUF MAIN33C; 332: C1Y=EHC0(1) MAIN33C; 333: C1Y=EHC0(NTY) MAIN33C; 334: C MAIN33C; 335: C MAIN33G; 336: C MAIN33G; 337: C=0.000 MAIN33G; 338: D0 47 1=2,N1Y MAIN33G; 338: D0 47 1=2,N1Y MAIN33G; 341: C=2.0019*C(1,J)*C(1,J)*U(J) MAIN33G; 342: 0=100.47 J=2,N1Z MAIN34G; 344: C MAIN34G; 342: 0=100.4000*C MAIN34G; 342: 0=100.4000*C MAIN34G; 344: C MAIN34G; 345: C CALCULATION CF THE TRUE CENTERLINE CONCENTRATIONS MAIN34G; 344: C MAIN34G; MAIN34G; 345: C CALCULATION CF THE TRUE CENTERLINE CONCENTRATIONS MAIN34G; 346: C MAIN34G; MAIN34G;	329:			DD 857 I=1,NTY	MAIN3290
331: 657 CONTINUF MAIN231C 322: C(Y=EHCO(1) MAIN332C 333: C1Y=EHCO(NTY) MAIN3333 334: C MAIN3330 335: C CALCULATION OF THE MASS RATE MAIN3360 337: C=0.000 MAIN3360 MAIN3360 337: C=0.000 MAIN3360 MAIN3370 338: D0 47 J=2.N12 MAIN3370 339: D0 47 J=2.N12 MAIN3350 340: 47 Q=0+wY(1)*wZ(J)*C(1,J)*u(J) MAIN3360 341: C=2.00*YMAX*(C1Y+D2Y+2.00*BETAY)*H*(D1Z+C27+2.00*BETAZ)*C MAIN3400 341: C=2.00*YMAX*(C1Y+D2Y+2.00*BETAY)*H*(D1Z+C27+2.00*BETAZ)*C MAIN3400 341: C=2.00*YMAX*(C1Y+D2Y+2.00*BETAY)*H*(D1Z+C27+2.00*BETAZ)*C MAIN3400 341: C=2.00*YMAX*(C1Y+D2Y+2.00*BETAZ)*C MAIN3420 341: C MAIN3420 MAIN3420 342: O=10CC.0.0/C6.0.00*C MAIN3450 MAIN3450 344: C MAIN3450 MAIN3450 347: RYC=(RETAY+C1Y+PV*ACTX/2.0C/YMAX)/(D1Y+D2Y+2.006*BETAY) MAIN3450 <td>330:</td> <td></td> <td></td> <td>CCO1=CCO1+YINTP(I)*EHCO(I)</td> <td>MAIN3307</td>	330:			CCO1=CCO1+YINTP(I)*EHCO(I)	MAIN3307
332: C(Y=EHCO(1) C1Y=EFCO(NTY) MAIN332C MAIN3333 334: C MAIN3333 335: C MAIN3335 336: C MAIN3350 337: C=0.°C0 MAIN3350 337: C=0.°C0 MAIN3350 338: D0 47 I=2,N1Y MAIN3350 339: D0 47 J=2,N1Z MAIN3350 341: C=0.°C0/C0/C0/C0/C0/C0/C0/C0/C0/C0/C0/C0/C0/C	331:		857	CONTINUE	MAIN331C
333: C1Y=EFCO(NTY) MAIN3333 334: MAIN3333 334: MAIN3343 335: C MAIN3343 336: D MAIN3350 337: C=0.C0 MAIN3350 337: D=0.47 I=2,N1Y MAIN3363 339: D0.47 J=2,N1Z MAIN3362 339: D0.47 J=2,N1Z MAIN3363 340: 47 Q=Q+twY(I)*kZ(J)*C(I,J)*U(J) MAIN3363 341: C=2.C1*YMAX*(D1Y+C2Y+2.C0*HETAY)*H*(D12+C27+2.LC*HETAZ)*C MAIN3403 342: ()=1CCC.DC/6C.DC*C MAIN34343 343: ACTX=XXMAX MAIN3420 344: C MAIN3452 344: C MAIN3454 347: RYC= (RETAY+C1Y+PV*ACTX/2.CC/YMAX)/(D1Y+D2Y+2.DC*BETAY) MAIN3454 346: C MAIN3452 347: RYC= (RETAY+C1Y+PV*ACTX/2.CC/YMAX)/(D1Y+D2Y+2.DC*BETAY) MAIN3463 349: PG 9 CEUY(J)=C.DC MAIN34523 350: IF(RYC.GE.I.DOC) IST=1 MAIN35333 351: CALL INTRF(I2,NTY,RYC,RTY,FAY,YINTP) <td>332:</td> <td></td> <td></td> <td>C(Y=EHCO(1)</td> <td>MAIN332C</td>	332:			C(Y=EHCO(1)	MAIN332C
334: C MAIN3341 335: C CALCULATION OF THE MASS RATE MAIN3341 336: D0 47 C=0.000 MAIN3370 338: D0 47 I=2.NIY MAIN3360 340: 47 C=0.4V(1)*VZ(J)*C(I,J)*U(J) MAIN3370 341: C=2.00*YMAX*(CIY+D2Y+2.00*BETAY)*H*(DIZ+027+2.00*BETAZ)*C MAIN3400 342: 0=10CC.0D/6C.0D*C MAIN3420 343: ACTX=XXMAX MAIN3430 344: C MAIN3433 345: C CALCULATION OF THE TRUE CENTERLINE CONCENTRATIONS MAIN3430 344: C MAIN3450 MAIN3450 347: RYC=(RETAY+DIY+PY*ACTX/2.0C/YMAX)/(DIY+D2Y+2.00*BETAY) MAIN3450 347: RYC=(RETAY+DIY+PY*ACTX/2.0C/YMAX)/(DIY+D2Y+2.00*BETAY) MAIN3462 349: D0 859 J=1.NTZ MAIN3450 349: D0 859 J=1.NTZ MAIN3450 350: IF(RYC.GE.1.0DC) IST=1 MAIN350 351: CALL INTFF(12.NTY, RYC, RTY, FAY, YINTP) MAIN351 MAIN3523 352: D0 </td <td>333:</td> <td></td> <td></td> <td>C1Y=EHCO(NTY)</td> <td>MAIN3330</td>	333:			C1Y=EHCO(NTY)	MAIN3330
335: C CALCULATION OF THE MASS RATE MAIN3350 336: C MAIN3360 337: C=0.*CO MAIN3370 338: D0 47 J=2,NIY MAIN3360 340: 47 Q=Q+WY(I)*bc(J)*C(I,J)*U(J) MAIN3360 341: C=2.CO*YMAX*(C1Y+D2Y+2.CO*BETAY)*H*(D1Z+C27+2.UC*BETAZ)*C MAIN3400 341: G=0.CC.DC/CC.OC*C MAIN3420 342: ACTX=X*XMAX MAIN3420 344: C MAIN3430 345: C CALCULATION OF THE TRUE CENTERLINE CONCENTRATIONS MAIN3460 344: C MAIN3460 MAIN3460 347: RYC=(RETAY+C1Y+PV*ACTX/2.DC/YMAX)/(D1Y+D2Y+2.D0*BETAY) MAIN3460 347: RYC=(RETAY+C1Y+PV*ACTX/2.DC/YMAX)/(D1Y+D2Y+2.D0*BETAY) MAIN3460 349: D0 859 J=1,NTZ MAIN3450 350: IF(RYC.GE.1.DOC) IST=1 MAIN3500 351: CALL INTRF(12,NTY,RYC,RTY,FAY,YINTP) MAIN3520 351: CALL INTRF(12,NTY,RYC,RTY,FAY,YINTP) MAIN3520 351: CALL INTRF(12,NTY,RYC,RTY,FAY,YINTP) MAIN3520 355: APYC=PV*ACTX MAIN3557 </td <td>334:</td> <td>С</td> <td></td> <td></td> <td>MAIN3347</td>	334:	С			MAIN3347
336: C MAIN3360 337: C=0.fC0 MAIN3370 338: D0 47 I=2,NIY MAIN3280 39: D0 47 J=2,NIZ MAIN3400 341: C=2.C0*YMAX*(CIY+C2Y+2.C0*BETAY)*H*(D1Z+C27+2.UC*BETAZ)*C MAIN3400 341: Q=1CCf.0C/6C.0C*C MAIN3410 342: Q=1CCf.0C/6C.0C*C MAIN3420 344: C MAIN3440 345: C CALCULATION CF THE TRUE CENTERLINE CONCENTRATIONS MAIN3450 346: C MAIN3460 MAIN3460 347: RYC=(RETAY+CIY+PV*ACTX/2.DC/YMAX)/(D1Y+D2Y+2.D0*BETAY) MAIN3460 347: D0 859 J=1,NTZ MAIN3480 349: D0 859 J=1,NTZ MAIN3480 349: PF5 CECUY(J)=C.DC MAIN3480 349: D0 859 J=1,NTZ MAIN3480 350: IF(RYC.GE.1.0DC) IST=1 MAIN3500 351: CALL INTFF(12,NTY,RYC,RTY,FAY,YINTP) MAIN3520 351: D0 86C J=1,NTZ MAIN3530 354: 661 CECUY(J)+YINTP(I)*C(I,J) MAIN3530 355: APYC=PV*ACTX MAIN3557	335:	С		CALCULATION OF THE MASS RATE	MAIN3350
337: C=0.CD MAIN3370 338: D0 47 I=2,NIY MAIN3280 339: D0 47 J=2,NIZ MAIN3280 340: 47 C=0+WY(I)*WZ(J)*C(I,J)*U(J) MAIN3400 341: C=2.CD*YMAX*(C1Y+C2Y+2.CO*BETAY)*H*(D1Z+C27+2.UC*BETAZ)*C MAIN3400 341: C=2.CD*YMAX*(C1Y+C2Y+2.CO*BETAY)*H*(D1Z+C27+2.UC*BETAZ)*C MAIN3400 342: ()=1CCC.DC/6C.DC*C MAIN3420 343: ACTX=X*XMAX MAIN3430 344: C MAIN3450 345: C CALCULATION OF THE TRUE CENTERLINE CONCENTRATIONS MAIN3450 346: C MAIN3460 MAIN3450 347: RYC=(RETAY+C1Y+PV*ACTX/2.DC/YMAX)/(D1Y+D2Y+2.D0*BETAY) MAIN3470 349: D0 859 J=1,NTZ MAIN3460 MAIN3480 349: D0 859 J=1,NTZ MAIN3490 MAIN3480 MAIN3480 350: IF(RYC.GE.1.0DC) IST=1 MAIN3500 MAIN3511 MAIN3520 MAIN3520 MAIN3520 MAIN3520 MAIN3520 MAIN3520 MAIN3520 MAIN3520 MAIN3520 MAIN3540 MAIN3550 MAIN3550 MAIN3550 MAIN3550 MAIN3550	336:	С			MA IN 3360
338: D0 47 I=2,NIY MAIN336C 339: D0 47 J=2,NIZ MAIN3390 340: 47 Q=Q+WY(I)*WZ(J)*C(I,J)*U(J) MAIN3400 341: C=2.C0*YMAX*(CIY+D2Y+2.C0*BETAY)*H*(D1Z+C27+2.UC*BETAZ)*C MAIN3400 342: O=1CCC,DC/6C.DC*0 MAIN3420 344: C MAIN3420 345: C CALCULATION OF THE TRUE CENTERLINE CONCENTRATIONS MAIN3450 346: C MAIN3470 347: RYC=(RETAY+CIY+PV*ACTX/2.DC/YMAX)/(D1Y+D2Y+2.D0*BETAY) MAIN3450 349: D0 859 J=1,NTZ MAIN3460 349: PFS CECUY(J)=C.DC MAIN3480 349: PFS CECUY(J)=C.DC MAIN3480 350: IF(RYC.0E.1.0DC) IST=1 MAIN3490 351: CALL INTRF(12,NTY,RYC,RTY,FAY,YINTP) MAIN3500 352: D0 %C J=1,NTZ MAIN3520 353: C0 86C I=1,NTY MAIN3530 354: %60 CECUY(J)=CECOY(J)+YINTP(I)*C(I,J) MAIN3530 354: %60 CECUY(J)=CECOY(J)+YINTP(I)*C(I,J) MAIN3557 355: APYC=PV*ACTX MAIN3557 356: DU 859 I=1,NTZ	337:			C=0.000	MAIN3370
339: D0 47 J=2,NIZ MAIN339C 340: 47 Q=Q+WY(I)*WZ(J)*C(I,J)*U(J) MAIN3400 341: Q=2.CD*YMAX*(CIY+C2Y+2.CD*BETAY)*H*(DIZ+C27+2.UC*BETAZ)*C MAIN3400 342: Q=1CCC.DC/GC.DC*C MAIN342C 343: ACTX=X*MAX MAIN342C 344: C MAIN3435 344: C MAIN345 345: C CALCULATION OF THE TRUE CENTERLINE CONCENTRATIONS MAIN345 346: C MAIN345 347: RYC=(RETAY+CIY+PV*ACTX/2.DC/YMAX)/(D1Y+D2Y+2.D0*BETAY) MAIN345 347: RYC=(RETAY+CIY+PV*ACTX/2.DC/YMAX)/(D1Y+D2Y+2.D0*BETAY) MAIN3460 347: RYC=(RETAY+CIY+PV*ACTX/2.DC/YMAX)/(D1Y+D2Y+2.D0*BETAY) MAIN3460 347: RYC=(RETAY+CIY+PV*ACTX/2.DC/YMAX)/(D1Y+D2Y+2.D0*BETAY) MAIN3460 347: D0 859 J=1,NTZ MAIN3460 349: PF5 CECUY(J)=C.DC MAIN3500 350: IF(RYC.GE.1.DC) IST=1 MAIN3500 MAIN351.J 351: CALL INTRF(I2,NTY,RYC,RTY,FAY,YINTP) MAIN351.J MAIN3520 353: CD 86C I=1,NTZ MAIN3557 MAIN3557	338:			DO 47 I=2,N1Y	MAIN338C
340: 47 Q=Q+WY(I)*WZ(J)*C(I,J)*U(J) MAIN3400 341: G=2.CO*YMAX*(C1Y+C2Y+2.CO*BETAY)*H*(D1Z+C27+2.CC*BETAZ)*C MAIN3410 342: O=1CCC.DC/6C.DC*C MAIN3420 343: ACTX=X*XMAX MAIN3420 344: C MAIN3430 345: C CALCULATION OF THE TRUE CENTERLINE CONCENTRATIONS MAIN3430 346: C MAIN3450 347: RYC=(RETAY+C1Y+PV*ACTX/2.CC/YMAX)/(D1Y+D2Y+2.DG*BETAY) MAIN3450 349: D0 859 J=1,NTZ MAIN3460 349: PFS CECUY(J)=COC MAIN3460 349: PFS CECUY(J)=COC MAIN3490 350: IF(RYC.GE.1.0DC) IST=1 MAIN3500 351: CALL INTRF(12,NTY,RYC,RTY,FAY,YINTP) MAIN3500 352: D0 %C J=1,NTZ MAIN3500 353: CU 86C I=1,NTZ MAIN3500 354: %600 CECUY(J)=CECUY(J)+YINTP(I)*C(I,J) MAIN3550 355: APYC=PV*ACTX MAIN3550 356: DU 859 I=1,NTZ MAIN3550 357: CC02=CC02+ZINTP(I)*CECO(I) MAIN3570 357: CC02=CC02+ZINTP(I)*CECO(I)	339:			DO 47 J=2,N1Z	MAIN3390
341: C=2.CD*YMAX*(CIY+C2Y+2.CO*BETAY)*H*(D1Z+C27+2.UC*BETAZ)*C MAIN341C 342: O=1CCC.DC/6C.DC*C MAIN342C 343: ACTX=X*XMAX MAIN3430 344: C MAIN3430 345: C CALCULATION OF THE TRUE CENTERLINE CONCENTRATIONS MAIN3450 346: C MAIN3450 347: RYC=(RETAY+CIY+PV*ACTX/2.DC/YMAX)/(D1Y+D2Y+2.D0*BETAY) MAIN3470 348: D0 859 J=1,NTZ MAIN349C 349: D0 859 J=1,NTZ MAIN349C 349: PFS CECUY(J)=C.DC MAIN349C 350: IF(RYC.GE.I.ODC) IST=1 MAIN3500 351: CALL INTRF(12,NTY,RYC,RTY,FAY,YINTP) MAIN351J 352: D0 %C J=1,NTZ MAIN3520 353: CD 86C I=1,NTZ MAIN3530 354: %600 CECUY(J)+YINTP(I)*C(I,J) MAIN3540 355: APYC=PV*ACTX MAIN3550 356: DU 859 I=1,NTZ MAIN3560 357: CC02=CC02+ZINTP(I)*CECO(I) MAIN3560 357: CC02=CC02+ZINTP(I)*CECO(I) MAIN3570 357: CC02=CC02+ZINTP(I)*CECOY(J) MAIN357	340:		47	Q = Q + WY(I) + WZ(J) + C(I, J) + U(J)	MAIN3400
342: 0=1CCf.DC/6C.DC*C MAIN3420 343: ACTX=X*XMAX MAIN3433 344: C MAIN3433 345: C CALCULATION OF THE TRUE CENTERLINE CONCENTRATIONS MAIN345. 346: C MAIN345. MAIN345. 347: RYC=(RETAY+C1Y+PV*ACTX/2.DC/YMAX)/(D1Y+D2Y+2.D0*BETAY) MAIN345. 347: DO 859 J=1,NTZ MAIN3463 349: DO 859 J=1,NTZ MAIN3460 349: PFS CECUY(J)=C.DC MAIN3460 350: IF(RYC.GE.1.0DC) IST=1 MAIN3462 351: CALL INTRF(12,NTY,RYC,RTY,FAY,YINTP) MAIN3500 351: CALL INTRF(12,NTY,RYC,RTY,FAY,YINTP) MAIN351. 352: DO 86C J=1,NTZ MAIN3523 353: CD 86C I=1,NTY MAIN3543 354: & 60 CECUY(J)=CECOY(J)+YINTP(I)*C(I,J) MAIN3543 355: APYC=PV*ACTX MAIN3547 356: DU 859 I=1,NTZ MAIN3567 357: CCD2=CC02+ZINTP(I)*CECOY(J) MAIN3570 356: DU 859 I=1,NTZ MAIN3570 357: CCD2=CC02+ZINTP(I)*CECOY(I) MAIN3	341:			G=2.C0*YMAX*(C1Y+C2Y+2.C0*BETAY)*H*(D1Z+C27+2.CG*BETAZ)*G	MAIN341C
343: ACTX=X*XMAX MAIN3433 344: C MAIN3451 345: C CALCULATION OF THE TRUE CENTERLINE CONCENTRATIONS MAIN3451 346: C MAIN3452 MAIN3452 346: C MAIN3452 MAIN3452 347: RYC=(RETAY+C1Y+PV*ACTX/2.0C/YMAX)/(D1Y+D2Y+2.00*BETAY) MAIN3463 348: D0 859 J=1,NTZ MAIN3463 349: PF9 CECUY(J)=C.0C MAIN3480 349: PF9 CECUY(J)=C.0C MAIN3480 350: IF(RYC.GE.1.0DC) IST=1 MAIN3480 351: CALL INTRF(12,NTY,RYC,RTY,FAY,YINTP) MAIN3503 351: CALL INTRF(12,NTY,RYC,RTY,FAY,YINTP) MAIN351.3 352: D0 %6C J=1,NTZ MAIN3523 353: C0 %6C J=1,NTZ MAIN3523 354: %60 CECUY(J)=CECUY(J)+YINTP(I)*C(I,J) MAIN3540 355: APYC=PV*ACTX MAIN3557 356: DU 859 I=1,NTZ MAIN3557 357: CCU2=CCU2+ZINTP(I)*CECU(I) MAIN3579 357: CCU2=CCU2+ZINTP(I)*CECU(I) MAIN3579	342:			Q = 100.00 / 60.00 * 0	MAIN3420
344: C MAIN3447 345: C CALCULATION OF THE TRUE CENTERLINE CONCENTRATIONS MAIN3450 346: C MAIN3451 MAIN3452 346: C MAIN3463 MAIN3451 347: RYC=(RETAY+C1Y+PV*ACTX/2.0C/YMAX)/(D1Y+D2Y+2.00*BETAY) MAIN3463 347: D0 859 J=1,NTZ MAIN3473 348: D0 859 J=1,NTZ MAIN3480 349: PF9 CECUY(J)=C.0C MAIN3480 350: IF(RYC.GE.1.0DC) IST=1 MAIN3500 351: CALL INTRF(12,NTY,RYC,RTY,FAY,YINTP) MAIN3513 352: D0 96C J=1,NTZ MAIN3523 353: C0 86C I=1,NTZ MAIN3523 354: 867 CECUY(J)+CECOY(J)+YINTP(I)*C(I,J) MAIN3547 355: APYC=PV*ACTX MAIN3547 356: DU 859 I=1,NTZ MAIN3567 357: CC02=CC02+ZINTP(I)*CECO(I) MAIN3579 356: DU 859 I=1,NTZ MAIN3567 357: CC02=CC02+ZINTP(I)*CECO(I) MAIN3579	343:			ACTX = X * XMAX	MAIN3430
345: C CALCULATION OF THE TRUE CENTERLINE CONCENTRATIONS MAIN3450 346: C MAIN3460 347: RYC=(RETAY+CIY+PV*ACTX/2.0C/YMAX)/(DIY+D2Y+2.00*BETAY) MAIN3460 349: D0 859 J=1,NTZ MAIN3490 349: PF9 CECUY(J)=C.0C MAIN3490 350: IF(RYC.GE.1.0DC) IST=1 MAIN3500 351: CALL INTRF(12,NTY,RYC,RTY,FAY,YINTP) MAIN351J 352: D0 860 J=1,NTZ MAIN3520 353: D0 860 J=1,NTZ MAIN3530 354: %60 CECUY(J)=CECUY(J)+YINTP(I)*C(I,J) MAIN3540 355: APYC=PV*ACTX MAIN3557 356: DU 859 I=1,NTZ MAIN3560 357: CCD2=CCU2+ZINTP(I)*CECO(I) MAIN3560 357: CCD2=CCU2+ZINTP(I)*CECUY(J) MAIN3560	344:	С			MAIN3447
346: C MAIN3462 347: RYC=(RETAY+C1Y+PV*ACTX/2.DC/YMAX)/(D1Y+D2Y+2.DG*BETAY) MAIN3470 349: D0 859 J=1,NTZ MAIN348C 349: PF9 CECUY(J)=C.DC MAIN349C 350: IF(RYC.GE.1.0DC) IST=1 MAIN3500 351: CALL INTRF(12,NTY,RYC,RTY,FAY,YINTP) MAIN351, 352: D0 96C J=1,NTZ MAIN3520 353: C0 86C I=1,NTZ MAIN3520 354: 667 CECUY(J)=CECOY(J)+YINTP(I)*C(I,J) MAIN3547 355: APYC=PV*ACTX MAIN3567 356: DU 859 I=1,NTZ MAIN3567 357: CC02=CC02+ZINTP(I)*CECO(I) MAIN3567 358: CC03=CC13+ZINTP(I)*CECO(I) MAIN3582	345:	С		CALCULATION OF THE TRUE CENTERLINE CONCENTRATIONS	MAIN345L
347: RYC=(RETAY+C1Y+PV*ACTX/2.DC/YMAX)/(D1Y+D2Y+2.D0*BETAY) MAIN3470 349: D0 859 J=1,NTZ MAIN348C 349: PF9 CECUY(J)=C.DC MAIN349C 350: IF(RYC.GE.1.0DC) IST=1 MAIN3500 351: CALL INTRF(12,NTY,RYC,RTY,FAY,YINTP) MAIN351J 352: DO 86C J=1,NTZ MAIN3520 353: CO 86C I=1,NTY MAIN3520 354: 860 CECUY(J)=CECOY(J)+YINTP(I)*C(I,J) MAIN3540 355: APYC=PV*ACTX MAIN3557 356: DU 859 I=1,NTZ MAIN3557 357: CC02=CC02+ZINTP(I)*CEC0(I) MAIN3570 358: CC03=CC02+ZINTP(I)*CEC0Y(I) MAIN3582	346:	С			MAIN3465
349: DO 859 J=1,NTZ MAIN348C 349: PES CECUY(J)=C.DC MAIN349C 350: IF(RYC.GE.1.0DC) IST=1 MAIN35C0 351: CALL INTRF(12,NTY,RYC,RTY,FAY,YINTP) MAIN351J 352: DO 96C J=1,NTZ MAIN3520 353: DO 86C I=1,NTZ MAIN3530 354: 860 CECUY(J)=CECOY(J)+YINTP(I)*C(I,J) MAIN3540 355: APYC=PV*ACTX MAIN3557 356: DU 859 I=1,NTZ MAIN3560 357: CCD2=CCO2+ZINTP(I)*CECD(I) MAIN3570 358: CCD3=CCC3+ZINTP(I)*CECDY(I) MAIN3582	347:			RYC=(BETAY+C1Y+PV*ACTX/2.DC/YMAX)/(D1Y+D2Y+2.DO*BETAY)	MAIN3470
349: PFS CECUY(J)=C.DC MAIN349C 350: IF(RYC.GE.1.ODC) IST=1 MAIN3500 351: CALL INTRF(12,NTY,RYC,RTY,FAY,YINTP) MAIN351J 352: DO R6C J=1,NTZ MAIN3520 353: CO 86C I=1,NTZ MAIN3530 354: 860 CECUY(J)=CECOY(J)+YINTP(I)*C(I,J) MAIN3540 355: APYC=PV*ACTX MAIN3550 356: DU 859 I=1,NTZ MAIN3560 357: CCD2=CCD2+ZINTP(I)*CECD(I) MAIN3570 358: CCD3=CCC3+ZINTP(I)*CECD(I) MAIN3580	349:			DO 859 J=1.NTZ	MAIN348C
350: IF(RYC.GE.1.ODC) IST=1 MAIN3500 351: CALL INTRF(12,NTY,RYC,RTY,FAY,YINTP) MAIN351, 352: DO R6C J=1,NTZ MAIN3520 353: CO 86C I=1,NTZ MAIN3530 354: 660 CECUY(J)=CECOY(J)+YINTP(I)*C(I,J) MAIN3540 355: APYC=PV*ACTX MAIN3550 356: DU 859 I=1,NTZ MAIN3560 357: CCD2=CCD2+ZINTP(I)*CECD(I) MAIN3570 358: CCD3=CCC3+ZINTP(I)*CECCY(I) MAIN3580	349:		pr.g	$CECUY(J) = C \cdot DC$	MAIN3490
351: CALL INTRF(12,NTY,RYC,RTY,FAY,YINTP) MAIN351, 352: DD 96C J=1,NTZ MAIN3523 353: DD 86C I=1,NTY MAIN3530 354: 867 CECUY(J)=CECOY(J)+YINTP(I)*C(I,J) MAIN3547 355: APYC=PV*ACTX MAIN3557 356: DU 859 I=1,NTZ MAIN3567 357: CCD2=CCD2+ZINTP(I)*CECD(I) MAIN3570 358: CCD3=CCC3+ZINTP(I)*CECCY(I) MAIN3582	350:			IF(RYC.GF.1.ODC) IST=1	MAIN3500
352: DO 96C J=1,NTZ MAIN3520 353: DO 86C I=1,NTY MAIN3530 354: 860 CECUY(J)=CECOY(J)+YINTP(I)*C(I,J) MAIN3540 355: APYC=PV*ACTX MAIN3550 356: DU 859 I=1,NTZ MAIN3560 357: CCD2=CCD2+ZINTP(I)*CECD(I) MAIN3570 358: CCD3=CCC3+ZINTP(I)*CECCY(I) MAIN3580	351:			CALL INTRE(12.NTY.RYC.RTY.EAY.YINTP)	MAIN351
353: DU 86C I=1,NTY 354: 860 CECUY(J)=CECOY(J)+YINTP(I)*C(I,J) 355: APYC=PV*ACTX 356: DU 859 I=1,NTZ 357: CCD2=CCD2+ZINTP(I)*CECD(I) 358: CCD3=CCC3+ZINTP(I)*CECCY(I)	352:			$D\Pi = 86C J=1 \cdot NT7$	MAIN 3520
354: 861 CECUY(J)=CECUY(J)+YINTP(I)*C(I,J) MAIN3540 355: APYC=PV*ACTX MAIN3550 356: DU 859 I=1,NTZ MAIN3560 357: CCD2=CCD2+ZINTP(I)*CECD(I) MAIN3570 358: CCD3=CCC3+ZINTP(I)*CECD(I) MAIN3580	353:			DD = 86C I = 1.NTY	MAIN3530
355: APYC=PV*ACTX MAIN3550 356: DU 859 I=1,NTZ MAIN3560 357: CCD2=CCD2+ZINTP(I)*CECD(I) MAIN3570 358: CCD3=CCC3+ZINTP(I)*CECCY(I) MAIN3580	354:		861	$C = C \cap Y(I) = C = C \cap Y(I) + Y = N = P(I) * C(I \cdot I)$	MAIN3540
356: DU 859 I=1,NTZ MAIN3560 357: CCD2=CCD2+ZINTP(I)*CECD(I) MAIN3570 358: CCD3=CCD3+ZINTP(I)*CECCY(I) MAIN3580	355:			$\Delta P Y C = P V * \Delta C T X$	MAINISSE
357: CCD2=CCD2+ZINTP(I)*CECD(I) MAIN3570 358: CCD3=CCC3+ZINTP(I)*CECCY(I) MAIN358C	356:			D(1 859 1=1.NT7)	MAIN3560
358: CCP3 = CCP3 + ZINTP(I) * CECPY(I) MAIN358C	357:			CCD2 = CCD2 + 7 INTP(I) * CFCD(I)	MAIN3570
	358:			CCO3 = CCC3 + ZINTP(I) * CECCY(I)	MAIN358C
359: 858 CENTINUE MAIN2590	359:		рьр	CONTINUE	MAIN259C

PACE

361: $C1/2 = CEOOY(NTZ)$ MAIN361362:EPS=CCO3*RATIOMAIN363363:CMAIN363364:CTEST FOR THE PLWE SPREAD BY CCMPARISON OF BOUNDARYMAIN364365:CCONCENTRATIONS WITH TPS (= C(TRUE CENTERLINE, EFFECTIVEMAIN365366:CIMISSION FEIGHT)*RATIOMAIN366367:C- IF OK, PRINT RESULTS AND ACVANCE INTEGRATION (12)MAIN367368:C- IF NOT, GET NEK INITIAL CONDITION AND INTEGRATE AGAINMAIN368370:IF(IOKYP.EC.2.AND.IOKYM.FC.2) GC TC 12MAIN373371:IOKZ=0MAIN373372:IOKZ=0MAIN373374:IF(UARIY.LT.I.CD-GA.AND.VAR2Y.LT.I.0D-0A) ICKY=1MAIN373374:IF(VARIY.LT.I.CD-GA.AND.VAR2Y.LT.I.PS) IOKY=1MAIN375376:IF(VARIY.LT.I.CD-GB.AND.(CIY).LT.EPS) IOKY=1MAIN376377:IF(IOKY.EC.I) GC IC 13MAIN377378:IF(DIY.LT.O.SDO-BETAY-1.CD-GB.AND.(CCY).GT.EPS)DIY=DIY+MAIN378379:ICCIY*CUL1.O.JB.AND.(CIY).GT.EPS) D2Y=C2Y+CC2Y*CMULYMAIN382381:IOKY=CMAIN383MAIN383384:13 CONTINUEMAIN373MAIN383384:13 CONTINUEMAIN361.MAIN383386:IF(ICYY.EC.1) IOKYP=1MAIN383386:IF((CIY).LT.O.CD) D2Y=D2Y-DD2Y*DMULY/2.5ECMAIN383389:ICKY=JMAIN386389:IF(ICKYF.EC.1) ICKYM=2MAIN383389:IF(ICWY.EC.1) ICKYM=2MAIN386389:IF(ICWY.EC.1) ICKYM	3c):	$C \Im Z = C F C C Y (1)$	MAIN3600
362: EPS=CC03*RATIO MAIN362 363: MAIN363 364: C TEST FOR THE PLUME SPREAD BY COMPARISON OF POUNCARY MAIN364 365: C CONCENTRATIONS WITH FPS (= C(TRUE CENTERLINE, EFFECTIVE MAIN363 366: C CONCENTRATIONS WITH FPS (= C(TRUE CENTERLINE, EFFECTIVE MAIN363 366: C IF (IOK PRINT RESULTS AND ACVANCE INTEGRATION (12) MAIN363 368: C IF (IOKYP.EC.2.AND.IOKYM.FC.2) GC TC 12 MAIN367 369: C MAIN363 MAIN373 371: IOK 2=0 MAIN373 MAIN373 372: IOK 2=0 MAIN373 MAIN373 373: IF (IOKYP.EC.2) AND. (CIY) .LT.EPS) IOKY=1 MAIN373 374: IF (VARIY.LT.1.CO-C8.AND.(CIY).LT.EPS) IOKY=1 MAIN373 374: IF (VARIY.LT.1.CO-C8.AND.(CIY).LT.EPS) IOKY=1 MAIN373 377: IF (IOKYP.EC.1) GC IC 13 MAIN373 378: IF (IOKYP.EC.1) GC IC 13 MAIN373 380: IF (IOKYP.EC.1) IOKYP=2 MAIN383 381: IOK*=C MAIN383 382: IF (ICKYP.EC.0) IOKYP=1 MAIN	361:	C1Z=CECOY(NTZ)	MAIN361(
363: C MAIN363 364: C TEST FOR THE PLUME SPREAD BY CCMPARISCN CF BCUNDARY MAIN363 364: C CONCENTRATIONS WITH FPS (= C(TRUE CENTERLINE,EFFECTIVE MAIN363 366: C CMISSION FEIGHT)*RATIC) MAIN366 367: C - IF OK, PRINT RESULTS AND ADVANCE INTEGRATION (12) MAIN366 369: C - IF NOT, CET NEW INITIAL CCNDITICN AND INTEGRATE AGAIN MAIN369 370: IF(IOKYP.EC.2.AND.IOKYM.FC.2) GC TC 12 MAIN373 371: IOKZ=0 MAIN373 372: IOKZ=0 MAIN373 373: IF((CY).LT.EPS.AND.(CIY).LT.EPS) IOKY=1 MAIN373 374: IF(VARIY.LT.I.CO-CR.AND.VARZY.LT.I.OD-R) ICKY=1 MAIN373 374: IF(VARY.EC.1) GC 1C 13 MAIN376 377: IF(IOKY.EC.1) GC 1C 13 MAIN376 379: ICCIY*CMUY MAIN376 379: ICCIY*CMUY MAIN378 381: IOKY-EC.1) IOKYP=2 MAIN373 382: IF(ICKYP.EC.1) IOKYP=1 MAIN383 384: 12 CONTINUE MAIN383 385: IF(ICKYP.EC.0) IO KYP=1 MAIN383 386: IF(ICKYP.	362:	EPS=CC03*RATIO	MAIN3620
364: C TEST FOR THE PLUME SPREAD BY CCMPARISON OF ECUNDARY MAIN364 365: C CONCENTRATIONS WITH FPS (= C(TRUE CENTERLINE, EFFECTIVE MAIN366 366: C - IF OK, PRINT RESULTS AND ADVANCE INTEGRATION (12) MAIN367 368: C - IF NOT, CET NEW INITIAL CONDITION AND INTEGRATE AGAIN MAIN369 369: C - IF (10KYP.EC.2.AND.IOKYM.FC.2) GC TC 12 MAIN372 371: IOKY=C MAIN372 MAIN373 372: IF((CYY).LT.EPS.AND.(CIY).LT.EPS) IOKY=1 MAIN373 374: IF(VARIY.LT.I.CD-G8.AND.VAR2Y.LT.I.OD-O8) ICKY=1 MAIN373 374: IF(VARIY.LT.I.CD-38.AND.(CIY).LT.EPS) IOKY=1 MAIN374 376: IF(VARYLT.L.OD-38.AND.(CIY).LT.EPS) IOKY=1 MAIN377 377: IF(IOKY.EC.1) GC IC 13 MAIN377 378: IF(VAR2Y.GT.I.OD-J8.AND.(CIY).LT.EPS) IOKY=1 MAIN377 379: ICDIYECUY MAIN377 381: IOKY=C MAIN378 382: IF(ICKYP.EC.1) IOKYP=2 MAIN382 383: IF(ICKYP.EC.0) IOKYP=1 MAIN382 384: 13 CONTINUE MAIN383 385: IF(ICKYP.EC.0) GO TO 1333 MAIN383 386: IF(CYC.GT.J.OC.AND.CIY.GT.O.D?) GO TO 1333 MAIN386 387: IF((ICKYP.EC.1) IOKYP=2 MAIN386 <tr< td=""><td>363:</td><td>C</td><td>MAIN363</td></tr<>	363:	C	MAIN363
365: C CONCENTRATIONS WITH FPS (= C(TRUE CENTERLINE, EFFECTIVE MAIN365 366: C MISSION HEIGHT)*RATIC) MAIN367 366: C IF (MS, PRINT RESULTS AND ADVANCE INTEGRATION (12) MAIN367 368: C IF NOT, CET NEW INITIAL CONDITION AND INTEGRATE AGAIN MAIN367 369: C MAIN367 MAIN367 370: IF(IOKYP.EC.2.AND.IOKYM.FC.2) GC TC 12 MAIN373 371: IOKZ=0 MAIN373 372: IOKZ=0 MAIN373 374: IF((CAR)Y.LT.EPS.AND.(CIY).LT.EPS) IOKY=1 MAIN373 374: IF(VARIY.LT.1.CD-CA.AND.VARZY.LT.1.0D-0A) ICKY=1 MAIN373 374: IF(VARIY.LT.1.CD-C8.AND.(CIY).LT.EPS) IOKY=1 MAIN374 375: IF(VARIY.LT.1.0D-38.AND.(CIY).LT.EPS) IOKY=1 MAIN375 376: IF(VARZY.LT.1.0D-38.AND.(CIY).LT.EPS) IOKY=1 MAIN376 377: IF(IDY.EC.1) GC IC 13 MAIN375 378: IF(IDY.LT.C.SDO-BETAY-1.(D-C8.AND.(CCY).GT.EPS)DIY=DIY+ MAIN375 379: ICCIY*CMULY MAIN375 MAIN375 384: I3 CONTINUE MAIN383 MAIN383 MAIN383 <td>364:</td> <td>C TEST FOR THE PLUME SPREAD BY COMPARISON OF BOUNDARY</td> <td>MAIN3643</td>	364:	C TEST FOR THE PLUME SPREAD BY COMPARISON OF BOUNDARY	MAIN3643
366: C CMISSION FEIGHT)*RATIC) MAIN366 367: C - IF OK, PRINT RESULTS AND ADVANCE INTEGRATION (12) MAIN367 368: C - IF NOT, GET NEW INITIAL CONDITION AND INTEGRATE AGAIN MAIN368 369: C MAIN367 MAIN367 370: IF(IOKYP.EC.2.AND.IOKYM.FC.2) GC TC 12 MAIN371 371: IOKZEO MAIN373 372: IF(COY).LT.EPS.AND.(CIY).LT.EPS) IOKY=1 MAIN373 374: IF(VARIY.LT.I.CD-G&AND.VAR2Y.LT.I.OD-O&) ICKY=1 MAIN373 374: IF(VARIY.LT.I.CD-G&AND.VAR2Y.LT.I.OD-O&) ICKY=1 MAIN373 376: IF(VARY.EC.1) GC IC 13 MAIN376 377: IF(IDIY.LT.F.SDG-BETAY-1.CD-C&AND.(CY).GT.EPS) DIY=1 MAIN377 378: IF(DIY.LT.G.SDG-BETAY-1.CD-C&AND.(CY).GT.EPS) DIY=1Y+ MAIN378 379: ICCIY*CMULY MAIN378 MAIN378 380: IF(IDKYP.EC.1) IOKYP=2 MAIN383 MAIN383 384: 13 CONTINUE MAIN383 MAIN383 MAIN383 386: IF(ICY.EC.0) GO TO 1333 MAIN386 MAIN386 387: IF(IIOKY.EC.0) GO TO 1333 MAIN386	365:	C CONCENTRATIONS WITH FPS (= C(TRUE CENTERLINE, EFFECTIVE	MAIN3650
367: C - IF OK, PRINT RESULTS AND ADVANCE INTEGRATION (12) MAIN367 368: C - IF NOT, CET NEW INITIAL CONDITION AND INTEGRATE AGAIN MAIN367 369: C MAIN367 MAIN367 370: IF(IOKYP.EC.2.AND.IOKYM.FC.2) GC TC 12 MAIN371 371: IOKZ=0 MAIN373 373: IF((CYM).LT.EPS.AND.(CIM).LT.EPS) IOKY=1 MAIN373 374: IF(VARIY.LT.I.CD-C8.AND.VAR2Y.LT.I.0D-08) ICKY=1 MAIN373 375: IF(VARIY.LT.I.CD-C8.AND.(CIM).LT.EPS) IOKY=1 MAIN375 376: IF(IOKY.EC.1) GC IC 13 MAIN376 377: IF(IOKY.EC.1) GC IC 13 MAIN376 378: IF(DIM.EC.1) OD-D8.AND.(CIM).GT.EPS) D2MEDIMEDIME MAIN376 379: ICCIMY.EC.1) OD-J8.AND.(CIM).GT.EPS) D2MEDIMEDIME MAIN377 378: IF(IOKY.EC.1) OD-J8.AND.(CIM).GT.EPS) D2MEDIMEDIME MAIN376 360: IF(IOKYP.EC.1) IOKYP=2 MAIN378 MAIN383 384: I3 CONTINUE MAIN383 MAIN383 MAIN383 386: IF(IOKYP.EC.0) GO TO 1333 MAIN386 MAIN386 387: IF(IOKY.EC.0) GO TO 1333 MAIN386 MA	366:	C EMISSION FEIGHT)*RATIC)	MAIN366
368: C - IF NOT, GET NEW INITIAL CONDITION AND INTEGRATE AGAIN MAIN368 369: C MAIN368 MAIN368 370: IF(IOKYP.EC.2.AND.IOKYM.FC.2) GC TC 12 MAIN370 371: IOKY=C MAIN371 372: IOKZ=O MAIN373 374: IF(COY).LT.EPS.AND.(CIY).LT.EPS) IOKY=1 MAIN373 374: IF(VARIY.LT.I.CD-C6.AND.VAR2Y.LT.I.OD-08) ICKY=1 MAIN373 376: IF(VARIY.LT.I.CD-C6.AND.VAR2Y.LT.I.OD-08) ICKY=1 MAIN373 376: IF(VARIY.LT.I.CD-C8.AND.(CIY).LT.EPS) IOKY=1 MAIN376 377: IF(IOKY.EC.1) GC 1C 13 MAIN376 377: IF(IOKY.EC.1) GC 1C 13 MAIN377 378: IF(IOKY.EC.1) GC 1C 13 MAIN377 379: ICCIY*CMULY MAIN378 380: IF(IOKYP.EC.1) IOKYP=2 MAIN378 381: IOKY=C MAIN383 384: 13 CONTINUE MAIN383 385: IF(ICKYP.EC.0) GO TO 1333 MAIN386 386: IF(C(CY).LT.CDO) DIY=DIY-DDIY*DMULY/2.5CC MAIN386 387: IF((CY).LT.O.CDO) DIY=DIY-DDIY*DMULY/2.5CC MAIN386	367:	C - IF OK, PRINT RESULTS AND ADVANCE INTEGRATION (12)	MAIN3670
369: C MAIN369 370: IF(IDKYP.EC.2.AND.IDKYM.FC.2) GC TC 12 MAIN370 371: IOKY=C MAIN370 371: IOKZ=O MAIN371 372: IOKZ=O MAIN373 373: IF((CAY).LT.EPS.AND.(CIY).LT.EPS) IOKY=1 MAIN373 374: IF(VARIY.LT.I.CD-C6.AND.VAR2Y.LT.I.OD-08) ICKY=1 MAIN374 375: IF(VARY.LT.I.OD-38.AND.(CIY).LT.EPS) IOKY=1 MAIN376 376: IF(IOKY.EC.1) GC 1C 13 MAIN377 378: IF(IOKY.EC.1) GC 1C 13 MAIN377 378: IF(IOY.LT.C.SDO-BETAY-1.CD-C8.AND.(CCY).GT.EPS)DIY=DIY+ MAIN377 378: IF(IOKY.EC.1) IOKYP=2 MAIN378 361: IOKY=C MAIN383 376: IF(ICKYP.EC.1) IOKYP=1 MAIN382 382: IF(ICKYP.EC.1) IOKYP=2 MAIN383 384: I3 CONTINUE MAIN383 386: IF(ICY.GT.J.DC.AND.CIY.GT.O.DO) GO TO 1333 MAIN386 386: IF((CIY).LT.C.CDO) IY=DIY-CDIY*CMULY/2.5CC MAIN387 388: IF(ICKYP.EC.1) ICKYM=2 MAIN386 3889: IF(ICKYP.EC.1) ICKYM=2 <td< td=""><td>368:</td><td>C - IF NOT, GET NEW INITIAL CONDITION AND INTEGRATE AGAIN</td><td>NAIN368(</td></td<>	368:	C - IF NOT, GET NEW INITIAL CONDITION AND INTEGRATE AGAIN	NAIN368(
37^: IF(I0KYP.EC.2.AND.IOKYM.FC.2) GC TC 12 MAIN37C 371: I0KY=C MAIN371 372: I0KZ=7 MAIN373 374: IF((CAY).LT.EPS.AND.(CIY).LT.EPS) IOKY=1 MAIN373 374: IF(VARIY.LT.I.CD-C8.AND.VAR2Y.LT.I.OD-08) ICKY=1 MAIN373 375: IF(VARIY.LT.I.CD-C8.AND.VAR2Y.LT.I.OD-08) ICKY=1 MAIN375 376: IF(VAR2Y.LT.I.OD-38.AND.(CIY).LT.EPS) IOKY=1 MAIN376 377: IF(ICKY.EC.I) GC IC I3 MAIN376 378: IF(DIY.T.O.SDO-BETAY-1.CD-C8.AND.(CCY).GT.EPS)DIY=DIY+ MAIN376 379: ICDIY*CMULY MAIN376 380: IF(ICKYP.EC.I) IOKYP=2 MAIN383 384: I2 CONTINUE MAIN383 385: IF(ICKYP.EC.O) GO TO 1333 MAIN385 386: IF((CCY).LT.C.COO)DIY=DIY-CDIY*CMULY/2.5CC MAIN386 388: IF((CCY).LT.C.COO)DIY=DIY-CDIY*DMULY/2.5CC MAIN388 389: ICKY=3 MAIN386 389: IF(ICKYM.EC.1) ICKYM=2 MAIN386 389: IF(ICKYM.EC.1) ICKYM=2 MAIN386 389: IF(ICKYM.EC.1) ICKYM=2 MAIN386 38	369:	C	MAIN3690
$371:$ $10KY=C$ $MAIN371$ $372:$ $10KZ=0$ $MAIN372$ $373:$ $IF((CYY) \cdot LT \cdot EPS \cdot AND \cdot (C1Y) \cdot LT \cdot EPS) IOKY=1$ $MAIN372$ $374:$ $IF(VAR1Y \cdot LT \cdot 1 \cdot CD - CB \cdot AND \cdot VAR2Y \cdot LT \cdot 1 \cdot 0D - 0B) ICKY=1$ $MAIN373$ $374:$ $IF(VAR1Y \cdot LT \cdot 1 \cdot CD - CB \cdot AND \cdot (C1Y) \cdot LT \cdot EPS) IOKY=1$ $MAIN375$ $375:$ $IF(VAR2Y \cdot LT \cdot 1 \cdot 0D - 0B \cdot AND \cdot (C1Y) \cdot LT \cdot EPS) IOKY=1$ $MAIN376$ $377:$ $IF(IOKY \cdot EC \cdot 1) GC IC I3$ $MAIN377$ $378:$ $IF(D1Y \cdot LT \cdot C \cdot 5D0 - BETAY - 1 \cdot CD - CB \cdot AND \cdot (CCY) \cdot GT \cdot EPS) D1Y = D1Y +379:ICC1Y * CMULYMAIN378390:IF(IOKY - EC \cdot 1) IOKYP = 2MAIN382381:IOKY = CMAIN382384:13 CONTINUEMAIN383384:13 CONTINUEMAIN383386:IF((CY) \cdot LT \cdot C \cdot CD0) D1Y = D1Y - CD1Y * CMULY/2 \cdot 5CCMAIN383389:IF((CY) \cdot LT \cdot C \cdot CD0) D1Y = D1Y - CD1Y * CMULY/2 \cdot 5CCMAIN383389:IF(ICKYP = 2)MAIN383389:IF(ICKYP = 2)MAIN383389:IF(ICKYP = 2)MAIN383389:IF(ICKYP = 2)MAIN383389:IF(ICKYP = 2)MAIN383389:IF(ICKYP = 2)MAIN383389:IF(ICKYP = 2)MAIN383380:IF(ICKYP = 2)MAIN392390:IF(IOKYP = 2) IOKYP = 2MAIN392390:IF(IOKYP = 2) IOKYP = 2MAIN382$	370:	IF(IOKYP.EC.2.AND.IOKYM.FC.2) GC TC 12	MAIN37C
372: IOK Z= 0 MAIN372 373: IF((C ∩ Y) + LT + EPS + ANC + (C1Y) + LT + EPS + IOK Y=1 MAIN373 374: IF((VAR1Y + LT + 1 + CD - C8 + AND + VAR2Y + LT + 1 + OD - 08 + ICK Y=1 MAIN374 375: IF(VAR1Y + LT + 1 + CD - C8 + AND + (C1Y) + LT + EPS + IOK Y=1 MAIN375 376: IF(VAR1Y + LT + 1 + CD - C8 + AND + (C1Y) + LT + EPS + IOK Y=1 MAIN375 376: IF(VAR1Y + LT + 0 - D - B + ANC + (C1Y) + LT + EPS + IOK Y=1 MAIN376 377: IF(IOKY + EC + 1) GC + C1 + 3 MAIN376 378: IF(D1Y + LT + C + SD0 - BETAY - 1 + (D - C8 + AND + (CCY) + GT + EPS + D1Y = D1Y + MAIN377 378: IF(D1Y + LT + C + SD0 - BETAY - 1 + (D - C8 + AND + (CCY) + GT + EPS + D1Y = D1Y + MAIN377 379: 1CC1Y + CMULY MAIN377 379: ICC1Y + CMULY MAIN376 381: IOK Y= C MAIN377 382: IF(ICKYP + EC + 1) IOK YP = 2 MAIN383 384: 13 CONTINUE MAIN383 384: 13 CONTINUE MAIN383 386: IF(ICKYP + EC + 1) IOK YP = 1 MAIN383 387: IF((ICKY) + C0 + O) O 1333 MAIN386 387: IF((C(Y) + LT + C + CDO) O 2Y = D 2Y + DD 2Y +	371:	I OK Y=C	MAIN371
373: IF((C^Y).LT.EPS.ANC.(CIY).LT.EPS) IOKY=1 MAIN373 374: IF(VARIY.LT.I.CD-C8.AND.VAR2Y.LT.I.OD-O8) ICKY=1 MAIN374 375: IF(VARIY.LT.I.CD-C8.AND.(CIY).LT.EPS) IOKY=1 MAIN375 376: IF(VAR2Y.LT.I.OD-38.ANC.(C'Y).LT.EPS) IOKY=1 MAIN375 376: IF(VAR2Y.LT.I.OD-38.ANC.(C'Y).LT.EPS) IOKY=1 MAIN375 377: IF(IOKY.EC.I) GC IC I3 MAIN376 377: IF(IOLY.LT.C.SDG-BETAY-1.CD-C8.AND.(CCY).GT.EPS)DIY=DIY+ MAIN377 378: IF(DY.LT.C.SDG-BETAY-1.CD-C8.AND.(CCY).GT.EPS)DIY=DIY+ MAIN376 379: ICLY*CMULY MAIN378 380: IF(IOKYP.EC.I) IOKYP=2 MAIN382 381: IOKY=C MAIN383 384: I3 CONTINUE MAIN383 385: IF(ICKYP.EC.O) IOKYP=1 MAIN383 386: IF(CCY).GT.O.DO.AND.CIY.GT.O.DO) GO TO 1333 MAIN386 387: IF((CLY).LT.C.CDO) DIY=DIY*CMULY/2.5CC MAIN388 388: IF((CLY).LT.O.CDO) D2Y=D2Y-DD2Y*DMLLY/2.5CC MAIN383 389: ICKY=J MAIN386 389: IF(ICKYM.EC.1) ICKYM=2 MAIN392 390: IF(IOKYM.EC.1) I	372:	IOK Z= C	MAIN372
374: IF(VARIY.LT.1.CD-C8.AND.VAR2Y.LT.1.0D-08) ICKY=1 MAIN374 375: IF(VARIY.LT.1.CD-08.AND.(CIY).LT.EPS) IOKY=1 MAIN375 376: IF(VAR2Y.LT.1.0D-08.ANC.(CIY).LT.EPS) IOKY=1 MAIN376 377: IF(IOKY.EC.1) GC IC I3 MAIN376 378: IF(D1Y.LT.C.5D0-BETAY-1.CD-C8.AND.(CCY).GT.EPS)D1Y=D1Y+ MAIN377 378: IF(D1Y.LT.C.5D0-BETAY-1.CD-C8.AND.(CCY).GT.EPS)D1Y=D1Y+ MAIN377 378: IF(D1Y.LT.C.5D0-BETAY-1.CD-C8.AND.(CCY).GT.EPS)D1Y=D1Y+ MAIN378 379: ICC1Y*CMULY MAIN379 360: IF(VAR2Y.GT.1.0D-J8.AND.(CIY).GT.EPS)D2Y=C2Y+CD2Y*CMULY MAIN382 381: IOKY=C MAIN383 382: IF(ICKYP.EC.1)IOKYP=2 MAIN383 384: I3 CONTINUE MAIN383 385: IF(IIOKY.EC.0)GO TO 1333 MAIN383 386: IF(CCY.GT.0.DC.AND.CIY.GT.0.DO)GO TO 1333 MAIN386 387: IF((CY).LT.C.COO)D1Y=D1Y-CD1Y*CMULY/2.5CC MAIN388 388: IF((CIY).LT.0.CD1)D2Y=D2Y-DD2Y*DMULY/2.5CC MAIN388 389: ICKY=3 MAIN389 390: ICKY=3 MAIN389	373:	IF((CAY).LT.EPS.ANC.(CIY).LT.EPS) IOKY=1	MAIN373
375: IF (VARIY.LT.1.CD-C8.AND.(CIY).LT.EPS) IOKY=1 MAIN375 376: IF (VAR2Y.LT.1.DD-J8.AND.(CIY).LT.EPS) IOKY=1 MAIN376 377: IF (IOKY.EC.1) GC 1C 13 MAIN377 378: IF (DIY.LT.C.5DO-BETAY-1.(D-C8.AND.(CCY).GT.EPS)DIY=DIY+ MAIN378 379: ICCIY*CMULY MAIN376 380: IF (VAR2Y.GT.1.OD-J8.AND.(CIY).GT.EPS) D2Y=C2Y+CD2Y*CMULY MAIN376 381: IOK Y=C MAIN382 381: IOK Y=C MAIN382 383: IF (ICKYP.EC.1) IOKYP=2 MAIN382 384: 13 CONTINUE MAIN383 385: IF (IICKY.EC.0) GO TO 1333 MAIN385 386: IF (CCY.GT.3.DC.AND.CIY.GT.0.DD) GO TO 1333 MAIN386 387: IF ((CIY).LT.C.CDD) D2Y=D2Y-DD2Y*DMLLY/2.5CC MAIN386 388: IF ((CIY).LT.0.CD1) D2Y=D2Y-DD2Y*DMLLY/2.5CC MAIN386 389: ICKY=3 MAIN385 MAIN385 389: IF (ICKYM.EC.1) ICKYM=2 MAIN386 389: IF (ICKYM.EC.1) ICKYM=2 MAIN386	374:	IF(VAR1Y.LT.1.CD-C8.AND.VAR2Y.LT.1.0D-08) ICKY=1	MAIN374
376: IF (VAR2Y.LT.1.0D-J8.ANC.(C.Y).LT.EPS) IOKY=1 MAIN376 377: IF (IOKY.EC.1) GC IC 13 MAIN377 378: IF (D1Y.LT.C.5D0-BETAY-1.CD-C8.AND.(CCY).GT.EPS)D1Y=D1Y+ MAIN377 379: ICC1Y*CMULY MAIN378 390: IF (VAR2Y.GT.1.0D-J8.AND.(C1Y).GT.EPS) D2Y=C2Y+CD2Y*CMULY MAIN379 381: IOK Y=C MAIN382 381: IOKY=C MAIN382 383: IF (ICKYP.EC.1) IOKYP=2 MAIN383 384: 13 CONTINUE MAIN383 385: IF (IIOKY.EC.0) GO TO 1333 MAIN385 386: IF (C.Y).LT.C.CD0)D1Y=D1Y-CD1Y*CMULY/2.5CC MAIN387 388: IF ((C1Y).LT.C.CD0)D1Y=D1Y-CD2Y*DMULY/2.5CC MAIN388 389: ICKY=J MAIN389 389: ICKY=J MAIN389	375:	IF (VAR1Y.LT.1.CD-C8.AND.(C1Y).LT.EPS) IOKY=1	MAIN375
377: IF(I0KY.EC.1) GC TC 13 378: IF(D1Y.LT.C.5D0-BETAY-1.CD-C8.AND.(CCY).GT.EPS)D1Y=D1Y+ 379: ICC1Y*CMULY 379: IF(VAR2Y.GT.1.0D-J8.AND.(C1Y).GT.EPS) D2Y=C2Y+CC2Y*CMULY 381: IOK.Y=C 381: IOK.Y=C 383: IF(ICKYP.EC.1) IOKYP=2 384: I3 CONTINUE 385: IF(IIOKY.EC.0) GO TO 1333 386: IF(CCY.GT.J.DC.AND.C1Y.GT.0.D0) GO TO 1333 386: IF(CCY).LT.C.COO)D1Y=D1Y+CD1Y*CMULY/2.5CC 388: IF((C1Y).LT.O.CD.) D2Y=D2Y-DD2Y*DMLLY/2.5CC 389: ICKY=J 389: ICKY=J 389: ICKY=J 380: IF(ICKYM.EC.1) ICKYM=2	376:	IF (VAR2Y.LT.1.DD-D8.ANC. (C)Y).LT.EPS) IOKY=1	MAIN376
378: IF(DIY.LT.C.5DC-BETAY-1.CD-C8.AND.(CCY).GT.EPS)DIY=DIY+ 379: 1CDIY*CMULY 379: IF(VAR2Y.GT.1.OD-J8.AND.(CIY).GT.EPS) D2Y=C2Y+CD2Y*CMULY 381: IF(VAR2Y.GT.1.OD-J8.AND.(CIY).GT.EPS) D2Y=C2Y+CD2Y*CMULY 381: IF(ICKYP.EQ.1) IOKYP=2 382: IF(ICKYP.EQ.1) IOKYP=1 384: I3 CONTINUE 385: IF(IICKYP.EQ.O) GO TO 1333 386: IF(COY.GT.J.DC.AND.CIY.GT.O.DO) GO TO 1333 387: IF(ICCY).LT.C.CDO)D1Y=D1Y-CD1Y*CMULY/2.5CC 388: IF((CIY).LT.O.CDO) D2Y=D2Y-DD2Y*DMULY/2.5CC 389: ICKY=J 390: ICKYP.J 389: IF(ICKYM.EQ.1) ICKYM=2	377:	IF(IOKY.EC.1) GC 1C 13	MAIN377
379: 1CC1Y*CMULY MAIN375 360: IF(VAR2Y.GT.1.0D-J8.AND.(C1Y).GT.EPS) D2Y=C2Y+CC2Y*CMULY MAIN380 381: IOKY=C MAIN380 381: IOKY=C MAIN381 382: IF(ICKYP.EQ.1) IOKYP=2 MAIN382 383: IF(ICKYP.EQ.0) IOKYP=1 MAIN383 384: 13 CONTINUE MAIN383 385: IF(IIOKY.EQ.0) GO TO 1333 MAIN385 386: IF(C^Y.GT.0.D0.AND.C1Y.GT.0.D0) GO TO 1333 MAIN385 387: IF((CLY).LT.C.CD0)D1Y=D1Y-CD1Y*CMULY/2.5CC MAIN387 388: IF((C1Y).LT.0.CD0) D2Y=D2Y-DD2Y*DMULY/2.5CC MAIN383 389: ICKY=J MAIN385 389: IF(IOKYM.EQ.1) ICKYM=2 MAIN39C	378:	IF(D1Y+LT+C+5D0+BETAY-1+CD+C8+AND+(CCY)+GT+EPS)D1Y=D1Y+	MAIN3780
360: IF(VAR2Y.GT.1.0D-J8.AND.(C1Y).GT.EPS) D2Y=D2Y+DD2Y*DMULY MAIN38C 381: IOKY=C MAIN381 382: IF(IGKYP.EQ.1) IOKYP=2 MAIN382 383: IF(ICKYP.EQ.0) IOKYP=1 MAIN383 384: 13 CONTINUE MAIN383 385: IF(IIOKY.EQ.0) GO TO 1333 MAIN385 386: IF(COY.GT.0.D0.AND.C1Y.GT.0.D0) GO TO 1333 MAIN386 387: IF((C1Y).LT.C.CD0)D1Y=D1Y-DD1Y*DMULY/2.5DC MAIN388 388: IF((C1Y).LT.0.CD0) D2Y=D2Y-DD2Y*DMULY/2.5DC MAIN389 389: ICKY=J MAIN389 390: IF(IOKYM.EQ.1) ICKYM=2 MAIN39C	379:		MAIN379
381: IOKY=C MAIN381 382: IF(IOKYP.EQ.1) IOKYP=2 MAIN382 383: IF(ICKYP.EQ.0) IOKYP=1 MAIN383 384: 13 CONTINUE MAIN383 385: IF(IIOKY.EQ.0) GO TO 1333 MAIN385 386: IF(COY.GT.D.DC.AND.CIY.GT.O.DO) GO TO 1333 MAIN385 387: IF((CUY).LT.C.CDO)DIY=DIY=DDIY=DDIY=25EC MAIN387 388: IF((CIY).LT.O.CDO) D2Y=D2Y=DD2Y=DMLLY/2.5EC MAIN388 389: ICKY=J MAIN385 390: IF(IOKYM.EC.1) ICKYM=2 MAIN39C	380:	$IE(VAR2Y_GT_1, 0D-J8_AND_(C1Y)_GT_EPS)$ $D2Y=C2Y+CC2Y*CMULY$	MAINBRO
382: IF(IOKYP.EQ.1) IOKYP=2 MAIN382 383: IF(ICKYP.EQ.1) IOKYP=1 MAIN383 384: 13 CONTINUE MAIN383 385: IF(IIOKY.EQ.0) GO TO 1333 MAIN385 386: IF(COY.GT.J.DO.AND.CIY.GT.O.DO) GO TO 1333 MAIN385 387: IF((CLY).LT.C.CDO)DIY=DIY-DDIY*DMULY/2.500 MAIN387 388: IF((CIY).LT.O.CDO) D2Y=D2Y-DD2Y*DMULY/2.500 MAIN388 389: ICKY=J MAIN389 390: IF(IOKYM.EQ.1) ICKYM=2 MAIN390	381:		NAIN3910
383: IF(ICKYP.E(.0)) IOKYP=1 MAIN383 384: 13 CONTINUE MAIN383 385: IF(IIOKY.EC.0) GO TO 1333 MAIN385 386: IF(COY.GT.J.OC.AND.CIY.GT.O.DO) GO TO 1333 MAIN385 387: IF((CLY).LT.C.CDO)DIY=DIY-CDIY*CMULY/2.5CC MAIN387 388: IF((CIY).LT.O.CDO) D2Y=D2Y+DMULY/2.5CC MAIN388 389: ICKY=J MAIN385 39C: IF(ICKYM.EC.1) ICKYM=2 MAIN39C	382:	$IE(IOKYP_EQ_1)$ IOKYP=2	MAIN3820
384: 13 CONTINUE MAIN384 385: IF(IIOKY.EQ.O) GO TO 1333 MAIN385 386: IF(COY.GT.J.OC.AND.CIY.GT.O.DO) GO TO 1333 MAIN385 387: IF((CLY).LT.C.CDO)DIY=DIY-DDIY*DMULY/2.500 MAIN387 388: IF((CIY).LT.O.CDO) D2Y=D2Y-DD2Y*DMULY/2.500 MAIN388 389: ICKY=J MAIN385 390: IF(IOKYM.EQ.1) ICKYM=2 MAIN390	383:	$IE(ICKYP_{\bullet}E(\bullet 0))$ $IOKYP=1$	MAIN383
385: IF(IIOKY.EQ.0) GO TO 1333 MAIN385 386: IF(COY.GT.J.DC.AND.CIY.GT.0.DO) GO TO 1333 MAIN386 387: IF((CLY).LT.C.CDO)DIY=DIY-CDIY*CMULY/2.5CC MAIN387 388: IF((CIY).LT.O.CDO) D2Y=D2Y-DD2Y*DMULY/2.5CC MAIN388 389: ICKY=J MAIN385 39C: IF(ICKYM.EC.I) ICKYM=2 MAIN39C	384:	13 CONTINUE	NATU384
386: IF(C^Y.GT.J.DC.AND.CIY.GT.O.D^) GO TO 1333 MAIN386 387: IF((CLY).LT.C.CDO)DIY=DIY=DDIY*EMULY/2.5EC MAIN387 388: IF((CIY).LT.O.CDO) D2Y=D2Y=DD2Y*DMULY/2.5EC MAIN388 389: ICKY=J MAIN386 39C: IF(ICKYM.EC.I) ICKYM=2 MAIN39C	385:	IE(II0KY,EG,D) = GO = TO = 1333	NATN3850
387: IF((CLY).LT.C.CD0)D1Y=D1Y-CD1Y*CMULY/2.5CC MAIN387 388: IF((C1Y).LT.O.CDO) D2Y=D2Y=DD2Y*DMULY/2.5CC MAIN388 389: ICKY=J MAIN385 39C: IF(ICKYM.EC.1) ICKYM=2 MAIN39C	386:	$IE(COY_{\bullet}GT_{\bullet})_{\bullet}DO_{\bullet}AND_{\bullet}CIY_{\bullet}GT_{\bullet}O_{\bullet}DO_{\bullet}) = GO_{\bullet}TO_{\bullet}1333$	MAIN386
388: IF((C1Y).LT.O.(DO)) D2Y=D2Y=DD2Y*DMULY/2.5EC MAIN388 389: IEKY=J MAIN385 39C: IF(IEKYM.EC.1) IEKYM=2 MAIN39C	387:	IE((C(Y), IT, C, CDQ)D)Y = DY = CDY + CDY + CMUY / 2,5CC	MAIN387
389: ICKY=J 39C: IF(ICKYM.EC.1) ICKYM=2 MAIN39C	388:	$IE((C1Y) T \cdot 1 \cdot CD \cdot 1) = D2Y = D2Y = DD2Y = D$	NATN3880
39C: IF(ICKYM.EC.1) ICKYM=2 MAIN39C	389:	ICKY=)	NAIN38S(
	390:	$IE(IDKYN_FC_1)$ $ICKYM=2$	MAIN39CO
	391:	$IE(IOKYM_EO_C)$ IOKYM=1	NAIN3910
392: 1323 CENTINUE	392:	1373 CONTINUE	NVIV.303
$353: IF((C^7)) IT_EPS_AND_A(C17) IT_EPS) ICK7=1 MAIN 393$	263.	I = I = I = I = E = A = C = C = C = C = C = C = C = C = C	MAINROR
$394: IE(VAR17_LT_1_CD-L8_AND_VAR27_LT_1_OD-CR) IE(K7=1) MAIN 394$	394:	$I = (V \land R \land I \land I \land C \land I \land C \land U \land C \land C$	MATN204
395: IF(VAR17.LT.1.CD-38.AND.(C17).LT.EPS) IOK7=1 NAIN395	395:	$I = \{V \in \mathbb{R} \mid Z = 1 \\ C = $	MAINA95

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396:	IF(VAR2Z.LT.1.CD-U8.AND.(CCZ).LT.EPS) ICKZ=1	MA IN3960
397:	IF(ICKY.EG.1.AND.IOKZ.EQ.1) GO TO 12	MAIN397)
398:	IF(D1Z.LT.SEL-BETAZ-1.(D-U8.AND.(CDZ).GT.EPS)D1Z=D1Z+	MAIN398C
399:	1001Z*DMULZ	MA IN 3990
400:	IF(VAR2Z.GT.1.CD-U8.ANU.(C1Z).GT.EPS) D2Z=C2Z+DD2Z*DMULZ	MAIN40JO
4.1:	$I \cap K Z = 0$	MAIN4C13
412:	133 CONTINUE	MAIN4C20
403:	IF(IOKY.EQ.1.AND.IOKZ.EQ.1) GG TC 12	MAIN4030
41,4:	IF(X.GE990-03) DMULY=2.D?	MAIN4040
465:	IF(X.GE99D-02) DMULY=6.DU	MAIN405C
406:	IF(X.GESSD-C1) DMULY=1C.DO	MA IN4967
407:	IF(X.GE99D-C3) DMULZ=4.DO	MAIN4070
438:	IF(X.GE990-02) CMULZ=12.00	MAIN4C8C
409:	IF(X.GE99D-C1) DMULZ=16.DC	MAIN4090
410:	IF(0.5CO-EETAY-CIY.LE.DDIY*DMULY) DDIY=(C.5DC-PETAY-CIY)/CMU	LY MAIN4100
411:	IF(1.DO-7.5D0-BETAY-C2Y.LE.CD2Y*DMULY)DC2Y=(1.D0-C.5DC-BĘTAY-	-D2Y)/MAIN411C
412:	ITMULY	MAIN412C
413:	IF(SEL-BETAZ-D1Z.LE.DD1Z*DMULZ) DD1Z=(SEL-PETAZ-D1Z)/DMULZ	MAIN4130
414:	IF(1.CO-SEL-BETAZ-D2Z.LE.CC2Z*DMULZ)CD2Z=(1.DC-SEL-BETAZ+D2Z)/ NAIN4140
415:	INMULZ	MAIN4150
416:	C	MAIN4160
417:	C CALCULATION OF NEW INITIAL CONDITION	MAIN4170
418:	C	MAIN418L
419:	X = XC	MAIN4190
423:	PRMT(1) = XC	MAIN4233
421:		MAIN4215
422:		MAIN422J
423:	76 DU 92 I=1,NY	MAIN4233
424:	J = I + I	MAIN4243
425	VIY=((DIY+D2Y+2.DV*BETAY)*RIY(I+1)+U19Y-U1Y)/(D19Y+C20Y+	MAIN4250
426:	12.00*BETAY)	MAIN426C
421:	IF(VIY-LI-I-JUN) GU IU 90	MAIN4273
423:	$\bigcup_{i=1}^{n} \bigcup_{j=1}^{n} \bigcup_{i=1}^{n} \bigcup_{j=1}^{n} \bigcup_{j=1}^{n} \bigcup_{j=1}^{n} \bigcup_{i=1}^{n} \bigcup_{j=1}^{n} \bigcup_{j$	MAIN428C
429:		MAIN4290
4 5/1:	90 IF(VIY+GT+C+)EC) GU TU 95	MAIN4357
431:	U(J,NUI)=0.000	MAIN431

432: CC TO 92 MAIN432C 433: 95 CALL INTRFIL2,NTY,VIY,RTY,FAY,YINTP) MAIN433C 434: C(J,NCI)=CC(1,NCI)*YINTP(1)+CC(NTY,NCI)*YINTP(NTY) MAIN434C 435: D0 93 K=1,NY MAIN436C 436: 93 C(J,NCI)=C(J,NCI)+YINTP(K+1)*CC(K+1,NCI) MAIN436C 437: 57 CCNTINUE MAIN436C 438: NCI='(CI+1) MAIN436C 439: IF(NCI.cT.NTZ) GD TO 955 MAIN436C 444: GD TO 96 MAIN4436C 441: 955 NCI=1 MAIN442C 442: ICO*C 00 42 MAIN442C 443: J=NCI+(I-1)*NY MAIN442C 444: VIZ=(ID12/DZ2+2.0C#8ETAZ) *RTZ(I+1)+CI0Z=CIZ)/(DI0Z+CZ0Z+ MAIN4442C 444: VIZ=(ID12/DZ2+2.0C#8ETAZ) *RTZ(I+1)+CI0Z=CIZ)/(DI0Z+CZ0Z+ MAIN4442C 444: VIZ=(ID12/DZ2+2.0C#8ETAZ) *RTZ(I+1)+CI0Z=CIZ)/(DI0Z+CZ0Z+ MAIN4442C 444: VIZ=(ID12/DZ2+2.0C#8ETAZ) *RTZ(I+1)+CI0Z=CIZ)/(DI0Z+CZ0Z+ MAIN4442C 444: VIZ=(ID12/DZ2+2.0C#8ETAZ) *RTZ(I+1)+CI0Z=CIZ)/(DI0Z+CZ0Z+ MAIN445C 444: IF(VIZ=CT.0-C) MAIN445C MAIN445C 451: CO <th></th> <th></th> <th></th> <th></th>				
433: 95 CALL INTRF[12,NTY,VIY,RTY,FAY,YINTP) MA1N433C 434: C(J,NCI)=CC(I,NCI)*VINTP(I)+CC(NTY,NCI)*VINTP(NTY) MA1N434C 435: D0 9; K=1,NY MA1N435C 436: 93 C(J,NCI)=C(J,NCI)+VINTP(K+1)*CC(K+1,NCI) MA1N435C 437: 57 CCMTINUE MA1N437C 438: NCI='ICI+1 MA1N436C 439: IF(NCI.GT.NTZ) GO TO 955 MAIN436C 444: 955 NCI=1 MAIN442C 442: J=NCI+(I-1)*NY MAIN442C 444: VIZ=(IO12+02+2+0C#BETAZ)*RTZ(I+1)+D10Z=D12)/(D102+D202+ MAIN444C 444: VIZ=(IO12+02+2+0C#BETAZ)*RTZ(I+1)+D10Z=D12)/(D102+D202+ MAIN445C 444: VIZ=(IO12+0-DC) GO TC 40 MAIN445C 444: GU TO 42 MAIN445C 444: GU TO 42 MAIN446C 445: I2_000*BETAZ) MAIN446C 446: IF(VIZ_CT_1,0-DC) GO TC 40 MAIN446C 447: P(J)=C.COC MAIN446C 452: AC (INTRP(I2,NTZ,VIZ,FIZ,FIZ,ZINTP) MAIN445C 452: AC (INTRP(I2,NTZ,VIZ,FIZ,FIZ,ZINTP) MAIN45C 454: D0 42 K=1,NZ </td <td>432:</td> <td></td> <td>CO TO 92</td> <td>MAIN4320</td>	432:		CO TO 92	MAIN4320
434: C(J,NCI)=C(1,NCI)*YINTP(1)+CC(NTY,NCI)*YINTP(NTY) MAIN4362 435: C0 9 K=1,NY MAIN4352 436: 93 C(J,NCI)=C(J,NCI)+YINTP(K+1)*CC(K+1,NCI) MAIN4362 437: 57 CCNTINUE MAIN4362 438: NCI=:CI+1 MAIN4363 439: IF(NCI.GT.NTZ) GO TO 955 MAIN4363 440: GO TO 96 MAIN4420 441: 955 ACI=1 MAIN4420 442: L^O^* CO 42 I=1,NZ MAIN4420 444: VIZ=((D1Z+D2Z+2.0C#BETAZ)*RTZ(I+1)+D10Z-C1Z)/(D10Z+C20Z+ MAIN4420 444: VIZ=((D1Z+D2Z+2.0C#BETAZ)*RTZ(I+1)+D10Z-C1Z)/(D10Z+C20Z+ MAIN4420 444: VIZ=((D1Z+D2Z+2.0C#BETAZ)*RTZ(I+1)+D10Z-C1Z)/(D10Z+C20Z+ MAIN4420 444: VIZ=(C0Z+C0C MAIN4420 444: VIZ=(C0Z MAIN4420 444: GU TO 42 MAIN4420 451: GU TO 42 MAIN4420 452: 45 CALL INTRP(12,NTZ,VIZ,RTZ,FAZ,ZINTP) MAIN4450 452: 45 CALL INTRP(12,NTZ,VIZ,RTZ,FAZ,ZINTP) MAIN4520 453: P(J)=C(NCI+1,1)*ZINTP(1)+C(NCI+1,NTZ)*ZINTP(NTZ) MAIN4520 45	433:	95	CALL INTRF(12,NTY,VIY,RTY,FAY,YINTP)	MAIN433C
435: D 92 K=1,NY MAIN4357 436: 93 C(J,NCI)=C(J,NCI)+YINTP(K+1)*CC(K+1,NCI) MAIN436C 437: 92 C(J,NCI)=C(J,NCI)+YINTP(K+1)*CC(K+1,NCI) MAIN436C 438: NCI=*(CI+1 MAIN436C 439: IF(NCI.GT.NTZ) GO TO 955 MAIN436C 444: GO TO 96 MAIN4420 442: I=NCI+(I=1)*KY MAIN4420 444: VIZ=((D12+02Z+2.0C*BETAZ)*RTZ(I+1)+C10Z=C12)/(D102+C20Z+ MAIN4420 444: VIZ=(CD12+02Z+2.0C*BETAZ)*RTZ(I+1)+C10Z=C12)/(D102+C20Z+ MAIN4420 444: VIZ=(CD12+02Z+2.0C*BETAZ)*RTZ(I+1)+C10Z=C12)/(D102+C20Z+ MAIN4420 444: VIZ=(CD12+02Z+2.0C*BETAZ)*RTZ(I+1)+C10Z=C12)/(D102+C20Z+ MAIN4450 444: VIZ=(CD12+02Z+2.0C*BETAZ)*RTZ(I+1)+C10Z=C12)/(D102+C20Z+ MAIN4450 444: VIZ=(CD12+02Z+2.0C*BETAZ)*RTZ(I+1)+C10Z=C12)/(D102+C20Z+ MAIN4450 444: IF(VIZ.CT.1.1.0D0) GO TC 40 MAIN4450 447: P(J)=C.COC MAIN4450 448: GO TO 42 MAIN4450 459: GO TO 42 MAIN4450 451: GO TO 42 MAIN4450 452: 45 CALL INTRP(12,NTZ,VI	434:		C(J, NCI) = CC(1, NCI) * YINTP(1) + CC(NTY, NCI) * YINTP(NTY)	MAIN4340
436: 93 Clj,NCl)=Clj,NCl)+YINTP(K+1)*CC(K+1,NCl) MAIN436C 437: 92 CGNTINUE MAIN436C 438: NCI='ICI+1 MAIN437C 439: IF(NCI.GT.NTZ) GO TO 955 MAIN436C 441: 955.NCI=1 MAIN436C 442: 1^^^ CG 42 I=1,NZ MAIN442C 443: J=NCI+(I=1)*NY MAIN442C 444: VIZ=(101Z+D2Z+2.DC*BETAZ)*RTZ(I+1)+D10Z-C12)/(D10Z+C20Z+ MAIN445C 444: VIZ=(101Z+D2Z+2.DC*BETAZ)*RTZ(I+1)+D10Z-C12)/(D10Z+C20Z+ MAIN445C 445: 12.^OD(#BETAZ) MAIN445C 446: IF(VIZ.LT.1.0C0) GO TC 40 MAIN447C 447: P(J)=C.C0C MAIN447C 448: GO TO 42 MAIN447C 449: 40 IF(VIZ.GT.0.0C0) GO TC 45 MAIN447C 451: C0 TO 42 MAIN445C 452: 45 CALL INTRP(12,NTZ,VIZ.FTZ.FAZ,ZINTP) MAIN452C 453: p(J)=C(NCI+1,1)*ZINTP(1)+C(NCI+1,NTZ)*ZINTP(NTZ) MAIN452C 453: p(J)=CNCINIL*Z MAIN455 454: D0 43 K=1,NZ MAIN45C 455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) <t< td=""><td>435:</td><td></td><td>CO 93 K=1,NY</td><td>MAIN4357</td></t<>	435:		CO 93 K=1,NY	MAIN4357
437: 57 CONTINUE MAIN437C 438: NCI='ICI+1 MAIN437C 439: IF(NCI.GT.NTZ) GD TD 955 MAIN436C 444: 955 NCI=1 MAIN44CC 442: I^O^C CD 42 I=1.NZ MAIN442C 444: J=NCI+(I-1)*NY MAIN442C 444: VIZ=(NDIX+DZ+2.DL*BETAZ)*RTZ(I+1)+C10Z-C12)/(D10Z+C20Z+ MAIN442C 444: VIZ=(NDIX+DZ+2.DL*BETAZ)*RTZ(I+1)+C10Z-C12)/(D10Z+C20Z+ MAIN443C 444: IF(VIZ.LT.1.0CD) GD TC 40 MAIN445D 444: GU TO 42 MAIN446C 447: P(J)=C.COC MAIN446C 448: GU TO 42 MAIN446C 447: P(J)=C.COC MAIN445D 457: P(J)=C.COC MAIN445D 457: GO TO 42 MAIN45C 452: 45 CALL INTRP(12.NTZ,VIZ.RTZ.FAZ.ZINTP) MAIN452C 453: P(J)=C(NCC MAIN452C 454: DU 43 K=1,NZ MAIN452C 455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) MAIN455C 455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) MAIN456C 456: 1F(NCI.G	436:	93	C(J,NCI)=C(J,NCI)+YINTP(K+1)*CC(K+1,NCI)	MAIN436C
438: NCI=VCI+1 MAIN430 439: IF(NCI.GT.NTZ) GO TO 955 MAIN4400 441: 955.ACI=1 MAIN4400 442: 1000 CO 42 I=1,NZ MAIN4420 444: VIZ=(01Z+02Z+2.0C*8FIAZ)*RTZ(I+1)+C10Z-C1Z)/(010Z+C20Z+ MAIN4420 444: VIZ=(01Z+02Z+2.0C*8FIAZ)*RTZ(I+1)+C10Z-C1Z)/(010Z+C20Z+ MAIN4440 445: 12.000*8ETAZ) MAIN4420 446: IF(VIZ.tT.1.1.0C0) GO TC 40 MAIN4460 447: P(J)=C.0C0 MAIN4460 448: GO TO 42 MAIN4450 449: 40 IF(VIZ.tT.1.0C0) GO TC 45 MAIN4450 449: GO TO 42 MAIN4450 451: GO TO 42 MAIN4450 452: 45 CALL INTRP(12,NTZ,VIZ,PTZ,FAZ,ZINTP) MAIN4520 454: D0 43 K=1,NZ MAIN4520 455: 42 CONTINUE MAIN4553 456: 42 CONTINUE MAIN4550 457: M (J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) MAIN4550 456: 42 CONTINUE MAIN4550 457: M (J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) MAIN4560 457:	437:	52	CONTINUE	MAIN4370
439: IF(NCI.GT.NTZ) GO TO 955 MAIN435C 440: GO TO 96 MAIN4400 441: 955.KCI=1 MAIN4410 442: 1000 CO 42 I=1.NZ MAIN4420 443: J=NCI+(I-I)*NY MAIN4420 444: VIZ=(D124022+2.000*BETAZ)*RTZ(I+1)+C102-C12)/(D102+C202+ MAIN4420 445: 12.000*BETAZ) MAIN44400 445: 19.00*BETAZ) MAIN44400 447: P(J)=0.0CO MAIN4460 447: P(J)=0.0D0 GO TC 40 MAIN4460 447: P(J)=0.0D0 GO TC 45 MAIN4460 447: P(J)=0.0D0 GO TC 45 MAIN4460 449: 40 IF(VIZ.GT.0.0D0) GO TC 45 MAIN4450 456: P(J)=C.COC MAIN4450 MAIN450 457: P(J)=C.(NCL MAIN450 MAIN450 456: GO TO 42 MAIN450 MAIN450 451: GO TO 42 MAIN450 MAIN450 452: 45 CALL INTRP(12,NTZ,VIZ,PTZ,FAZ,ZINTP) MAIN450 454: DO 43 K=1,NZ MAIN450 MAIN450 <	438:		NCI=NCI+1	MAIN4387
44C: GO TO 96 MAIN44C0 441: 955 NCI=1 MAIN4410 442: 1000 62 I=1,NZ MAIN4420 444: VIZ=((D12+D22+2.DC*BETAZ)*RTZ(I+1)+D10Z-D12)/(D102+C202+ MAIN4420 444: VIZ=((D12+D22+2.DC*BETAZ)*RTZ(I+1)+D10Z-D12)/(D102+C202+ MAIN44420 444: VIZ=((D12+D22+2.DC*BETAZ)*RTZ(I+1)+D10Z-D12)/(D102+C202+ MAIN44420 445: IF(VIZ.LT-1.0D0) GO TC 40 MAIN4450 446: IF(VIZ.CT.0.0D0) GO TC 40 MAIN4460 447: P(J)=C.CDC MAIN4460 449: 40 IF(VIZ.GT.0.0D0) GO TC 45 MAIN4460 449: 40 IF(VIZ.GT.0.0D0) GO TC 45 MAIN4450 451: GO TO 42 MAIN4450 MAIN450 452: 45 CALL INTRP(12,NTZ,VIZ,RTZ,FAZ,ZINTP) MAIN450 452: 45 CALL INTRP(12,NTZ,VIZ,RTZ,FAZ,ZINTP) MAIN4520 452: 47 P(J)=C(NCI+1,1)*ZINTP(1)+C(NCI+1,K+1) MAIN4520 455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) MAIN4520 456: GO TC 1000 MAIN450 MAIN450 457: MCI=NCI+1 MAIN	439:		IF(NCI.GT.NTZ) GD TD 955	MAIN439C
441: 955 ACI=1 MAIN4410 442: 1°0° CO 42 I=1,NZ MAIN4420 443: J=NCI+(I-1)*NY MAIN4420 444: VIZ=((D1Z+D2Z+2.DC*BETAZ)*RTZ(I+1)+D10Z-D1Z)/(D10Z+D20Z+2 MAIN4420 445: 12.000*BETAZ) MAIN4450 446: IF(VIZ+LT-1.0°C) GO TC 40 MAIN4460 447: P(J)=0.COC MAIN4460 448: GU TO 42 MAIN4480 449: 40 IF(VIZ.GT.0.000) GO TC 45 MAIN4480 450: P(J)=(.fOC MAIN4480 451: GO TO 42 MAIN4480 452: 45 CALL INTRP(12,NTZ,VIZ,RTZ,FAZ,ZINTP) MAIN4520 453: P(J)==C(NCI+1,I)*ZINTP(1)+C(NCI+1,NTZ)*ZINTP(NTZ) MAIN4520 454: DO 43 K=1,NZ MAIN450 455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) MAIN456C 457: NCI+NUE MAIN456C 457: GO TO 20 MAIN456C 457: C MAIN456C 456: IF(NCI.GT.NY) GO TO 20 MAIN456C 457: C MAIN456C 458: IF(NCI.GT.NY) GO TO 20 MAIN	440:		GO TO 96	MAIN44CC
442: 1°°° CO 42 I=1,NZ MAIN4420 443: J=NCI+(I-1)*NY MAIN4420 444: VIZ=((D12+D22+2.DC*BETAZ)*RTZ(I+1)+D10Z=C12)/(D10Z+C20Z+ MAIN4440 445: 12.°D0*BETAZ) MAIN4440 446: IF(VIZ.LT.1.°D°) GO TC 40 MAIN4460 447: P(J)=C.CDC MAIN4460 449: 40 IF(VIZ.GT.°.OD°) GO TC 45 MAIN4480 449: 40 IF(VIZ.GT.°.OD°) GO TC 45 MAIN4480 449: 40 IF(VIZ.GT.°.OD°) GO TC 45 MAIN4480 452: 45 CALL INTRP(12,NTZ,VIZ,FTZ,FAZ,ZINTP) MAIN450 452: 45 CALL INTRP(12,NTZ,VIZ,FTZ,FAZ,ZINTP) MAIN4520 453: P(J)=C(NCI+1,1)*ZINTP(1)+C(NCI+1,NTZ)*ZINTP(NTZ) MAIN4520 454: DU 43 K=1,NZ MAIN4550 455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) MAIN456C 457: NCI=NCI+1 MAIN456C MAIN456C 457: NCI=NCI+1 MAIN456C MAIN456C 459: GO TC 100C MAIN456C MAIN466C 461: C MAIN466C MAIN466C	441:	955	NC I = 1	MAIN4410
443: J=NCI+(I-1)*NY MAIN443C 444: VIZ=((D1Z+D2+2+DC*BETAZ)*RTZ(I+1)+DDZ+C1Z)/(D1CZ+C2CZ+ MAIN444CD 445: 12.*D0*BETAZ] MAIN445D 446: IF(VIZ+LT+1.*DC)) GO TC 4C MAIN446C 447: P(J)=C.CDC MAIN446C 448: GU TO 42 MAIN448C 449: 40 TE(VIZ.GT.*0.0C0) GO TC 45 MAIN448C 457: P(J)=C.CDC MAIN448C 452: 45 CALL INTRP(12,NTZ,VIZ,RTZ,FAZ,ZINTP) MAIN4520 453: P(J)=C(NCI+1,1)*ZINTP(1)+C(NCI+1,NTZ)*ZINTP(NTZ) MAIN4520 454: DO 43 K=1,NZ MAIN4550 455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,NTZ)*ZINTP(NTZ) MAIN456C 457: NCI=NCI+1 MAIN456C 459: GO TC 100C MAIN46	442:	1000	CO 42 I=1,NZ	MAIN4420
444: VIZ=((D1Z+D2Z+2.DC*BETAZ)*RTZ(I+1)+D10Z-C12)/(D10Z+C20Z+ MAIN4440 445: 12.0D0#BETAZ) MAIN4450 446: IF(VIZ.LT.1.0D0) G0 TC 40 MAIN446C 447: P(J)=C.CDC MAIN447C 448: G0 TO 42 MAIN448C 449: 40 IF(VIZ.GT.0.0D0) G0 TC 45 MAIN448C 450: P(J)=C.CDC MAIN45CO 451: G0 TO 42 MAIN45CO 452: 45 CALL INTRP(12,NTZ,VIZ,RTZ,FAZ,ZINTP) MAIN45CO 453: P(J)=C(NCI+1,1)*ZINTP(1)+C(NCI+1,NTZ)*ZINTP(NTZ) MAIN4520 454: D0 43 K=1,NZ MAIN450 455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) MAIN4550 456: 42 CONTINUE MAIN456C 457: NCI=NCI+1 MAIN456C 458: IF(NCI.GT.NY) CO TO 2C MAIN456C 459: G0 TC 100C MAIN467C 461: C MAIN467C 462: C MAIN467C 455: 12 CONTINUE MAIN4630 461: C PRINT AND STORE THE RESULTS MAIN467C 463: 10KYP=0 MAIN46	443:		J=NCI+(I-1)*NY	MAIN443C
445: 12.000*BETAZ) MAIN4450 446: IF(VIZ.LT.1.0.00) GO TC 40 MAIN4460 447: P(J)=C.CDC MAIN4470 448: GU TO 42 MAIN4480 449: 40 IF(VIZ.GT.0.000) GO TC 45 MAIN4480 451: GO TO 42 MAIN4500 452: 45 CALL INTRP(12,NTZ,VIZ,RTZ,FAZ,ZINTP) MAIN4520 453: P(J)=C(NCI+1,1)*ZINTP(1)+C(NCI+1,NTZ)*ZINTP(NTZ) MAIN4530 454: DO 43 K=1,NZ MAIN4540 455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) MAIN4560 456: QI)=QUYLINUE MAIN4560 457: NCI=NCI+1 MAIN4570 458: IF(NCI.GT.NY) CO TO 2C MAIN4580 459: GO TC 100C MAIN4580 460: C MAIN4580 461: C PRINT AND STORE THE RESULTS MAIN4600 462: C MAIN4620 463: 12 CONTINUE MAIN4620 464: IOKYP=0 MAIN4600 464: IOKYP=0 MAIN4620 465: IOKYM=0 MAIN4660 466:	444:		VIZ=((D1Z+D2Z+2.DC*BETAZ)*RTZ(I+1)+D10Z-C1Z)/(D10Z+C20Z+	MAIN4440
446: IF(VIZ.LT.1.0C0) G0 TC 40 MAIN446C 447: P(J)=C.CDC MAIN447C 448: G0 TO 42 MAIN448C 449: F(VIZ.GT.0.0C0) G0 TC 45 MAIN448C 457: P(J)=C.CDC MAIN45CO 457: GO TO 42 MAIN45CO 451: GO TO 42 MAIN452O 452: 45 CALL INTRP(12,NTZ,VIZ,RTZ,FAZ,ZINTP) MAIN452O 454: DO 42 K=1,NZ MAIN453O 454: DO 42 K=1,NZ MAIN454O 455: 43 P(J)=P(J)+ZINTP(1)+C(NCI+1,NTZ)*ZINTP(NTZ) MAIN454O 455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) MAIN454O 456: ACONTINUE MAIN456C 457: NCI=NCI+1 MAIN458O 458: IF(NCI.GT.NY) GO TO 2C MAIN458O 459: GO TC 100C MAIN46CO 460: C MAIN46CO 461: C PRINT AND STORE THE RESULTS MAIN4620 462: C MAIN4620 MAIN4640 465: IOKYP=0 MAIN4640 MAIN4640 466: C10Y=01Y MAI	445:		12.ºD0*BETAZ)	MAIN4450
447: P(J)=C.CDC MAIN447C 448: GU TU 42 MAIN448C 449: 40 IF(VIZ.GT.0.0C0) GD TC 45 MAIN448C 451: P(J)=C.CDC MAIN45CO 451: GU TU 42 MAIN451C 452: 45 CALL INTRP(12,NTZ,VIZ,RTZ,FAZ,ZINTP) MAIN4520 453: P(J)=C(NCI+1,1)*ZINTP(1)+C(NCI+1,NTZ)*ZINTP(NTZ) MAIN4530 454: DU 43 K=1,NZ MAIN456C 455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) MAIN456C 457: NCI=NCI+1 MAIN457C 458: IF(NCI.GT.NY) GU TU 2C MAIN4580 459: GU TC 100C MAIN458C 460: C MAIN456C 461: C PRINT AND STORE THE RESULTS MAIN462D 463: 12 CONTINUE MAIN462D 464: IOKYP=0 MAIN462D 464: IOKYP=0 MAIN462D 466: D10Y=D1Y MAIN467C	446:		IF(VIZ.LT.1.)CO) GO TC 40	MAIN446C
448: GU TO 42 MAIN448C 449: 40 IF(VIZ.GT.0.0D0) GD TC 45 MAIN448C 450: P(J)=C.FDC MAIN45CG 451: GO TO 42 MAIN45C 452: 45 CALL INTRP(12,NTZ,VIZ,RTZ,FAZ,ZINTP) MAIN4520 453: P(J)=C(NCI+1,1)*ZINTP(1)+C(NCI+1,NTZ)*ZINTP(NTZ) MAIN4520 454: DO 43 K=1,NZ MAIN4540 455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) MAIN4540 455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) MAIN4550 456: 42 CONTINUE MAIN456C 457: NCI=NCI+1 MAIN457C 458: IF(NCI.GT.NY) GO TO 2C MAIN457C 461: C PRINT AND STORE THE RESULTS MAIN462C 462: C MAIN462C MAIN462C 463: 12 CONTINUE MAIN4620 MAIN4620 464: IOK YP=0 MAIN4620 MAIN4642 465: IOK YP=0 MAIN4662 MAIN4662 466: CI Y=D1Y MAIN4662 MAIN4662	447:		$P(J) = C_{\bullet} CDC$	MAIN447C
449: 40 IF(VIZ.GT.0.0C0) GO TC 45 MAIN4490 450: P(J)=C.CDC MAIN45CO 451: GO TO 42 MAIN451C 452: 45 CALL INTRP(12,NTZ,VIZ,PTZ,FAZ,ZINTP) MAIN4520 453: P(J)=C(CCI+1,1)*ZINTP(1)+C(NCI+1,NTZ)*ZINTP(NTZ) MAIN4530 454: DO 43 K=1,NZ MAIN4540 455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) MAIN4550 456: 42 CONTINUE MAIN4550 457: NCI=NCI+1 MAIN4560 458: IF(NCI.GT.NY) CO TO 2C MAIN4580 459: GO TC 100C MAIN4580 459: GO TC 100C MAIN460C 461: C MAIN460C 463: 12 CONTINUE MAIN4600 464: IOKYP=0 MAIN4630 465: IOKYP=0 MAIN4640 466: C10Y=01Y MAIN4660	448:		GU TU 42	MAIN4480
45°: P(J)=C.CDC MAIN45CC 451: GO TO 42 MAIN451C 452: 45 CALL INTRP(12,NTZ,VIZ,RTZ,FAZ,ZINTP) MAIN452O 453: P(J)=C(NCI+1,1)*ZINTP(1)+C(NCI+1,NTZ)*ZINTP(NTZ) MAIN452O 454: DO 43 K=1,NZ MAIN455 D 455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) MAIN455 D 456: 42 CONTINUE MAIN455 D 457: NCI=NCI+1 MAIN457C 458: IF(NCI.GT.NY) CO TO 2C MAIN4580 459: GO TC 100C MAIN4620 460: C MAIN4610 461: C PRINT AND STORE THE RESULTS MAIN4620 463: 12 CONTINUE MAIN4620 MAIN4630 464: 10KYP=0 MAIN4640 MAIN4640 465: I0KYM=0 MAIN4660 MAIN4640 466: C10Y=D1Y MAIN4660 MAIN4640 466: C10Y=D1Y MAIN4670 MAIN4660	449:	40	IF(VIZ.GT.0.0C0) GO TC 45	MAIN445C
451: GO TO 42 MAIN451C 452: 45 CALL INTRP(12,NTZ,VIZ,RTZ,FAZ,ZINTP) MAIN4520 453: P(J)=C(NCI+1,1)*ZINTP(1)+C(NCI+1,NTZ)*ZINTP(NTZ) MAIN4530 454: DO 43 K=1,NZ MAIN4540 455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) MAIN4551 456: 42 CONTINUE MAIN4551 457: NCI=NCI+1 MAIN4560 458: IF(NCI.GT.NY) CO TO 2C MAIN4580 459: GO TC 100C MAIN459C 460: C MAIN460C 461: C PRINT AND STORE THE RESULTS MAIN4620 462: C MAIN4620 MAIN4640 463: 12 CONTINUE MAIN4640 MAIN4640 465: IOKYP=0 MAIN4640 MAIN4640 465: IOKYM=0 MAIN4640 MAIN4640 466: D10Y=D1Y MAIN466C MAIN466C 467: D20Y=D2Y MAIN467C MAIN467C	450:		$P(J) = C_{\bullet} C D C$	MAIN45CO
452: 45 CALL INTRP(12,NTZ,VIZ,RTZ,FAZ,ZINTP) MAIN4520 453: P(J)=C(NCI+1,1)*ZINTP(1)+C(NCI+1,NTZ)*ZINTP(NTZ)) MAIN4530 454: DD 43 K=1,NZ MAIN4540 455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1)) MAIN4550 456: 42 CONTINUE MAIN456C 457: NCI=NCI+1 MAIN457C 458: IF(NCI.GT.NY) GO TO 2C MAIN4580 459: GO TC 100C MAIN456C 460: C MAIN4620 461: LOKYP=0 MAIN4630 462: C MAIN4630 464: LOKYP=0 MAIN4650 465: LOKYM=0 MAIN4650 466: C10Y=01Y MAIN466C 467: D20Y=D2Y MAIN4670	451:		GO TO 42	MAIN4510
453: P(J)=C(NCI+1,1)*ZINTP(1)+C(NCI+1,NTZ)*ZINTP(NTZ) MAIN4530 454: DO 43 K=1,NZ MAIN4540 455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) MAIN4550 456: 42 CONTINUE MAIN456C 457: NCI=NCI+1 MAIN457C 458: IF(NCI.GT.NY) GO TO 2C MAIN4580 459: GO TC 100C MAIN456C 460: C MAIN467C 461: C PRINT AND STORE THE RESULTS MAIN4620 462: C MAIN4620 MAIN4630 464: IOK YP=0 MAIN4630 MAIN4630 465: IOK YM=0 MAIN4640 MAIN4640 466: C10Y=D1Y MAIN4650 MAIN4640 466: C10Y=D1Y MAIN466C MAIN466C 467: D20Y=D2Y MAIN4670 MAIN466C	452:	45	CALL INTRP(12,NTZ,VIZ,RTZ,FAZ,ZINTP)	MAIN4520
454: DD 43 K=1,NZ MAIN4540 455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) MAIN4550 456: 42 CONTINUE MAIN456C 457: NCI=NCI+1 MAIN457C 459: IF(NCI.GT.NY) CO TO 2C MAIN4580 459: GO TC 100C MAIN459C 460: C MAIN4610 462: C MAIN4610 463: 12 CONTINUE MAIN4620 464: IOKYP=0 MAIN4650 465: IOKYM=0 MAIN4650 466: C10Y=D1Y MAIN4660 466: C10Y=D1Y MAIN4670	453:		P(J)=C(NCI+1,1)*ZINTP(1)+C(NCI+1,NTZ)*ZINTP(NTZ)	MAIN4530
455: 43 P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1) MAIN455) 456: 42 CONTINUE MAIN456C 457: NCI=NCI+1 MAIN457C 458: IF(NCI.GT.NY) CO TO 2C MAIN4580 459: GO TC 100C MAIN459C 460: C MAIN4610 462: C MAIN4610 463: 12 CONTINUE MAIN4620 464: IOKYP=0 MAIN4630 465: IOKYM=0 MAIN4650 466: C10Y=D1Y MAIN4660 467: D20Y=D2Y MAIN4670	454:		DO 43 K=1,NZ	MA IN4540
456: 42 CONTINUE MAIN456C 457: NCI=NCI+1 MAIN457C 458: IF(NCI.GT.NY) CO TO 2C MAIN4580 459: GO TC 100C MAIN459C 460: C MAIN467C 461: C PRINT AND STORE THE RESULTS MAIN4610 462: C MAIN4620 MAIN4620 463: 12 CONTINUE MAIN4630 MAIN4640 464: IOK YP=0 MAIN4650 MAIN4650 466: C1 0Y=D1Y MAIN4650 MAIN4662 467: D20Y=D2Y MAIN467C MAIN467C	455:	43	P(J)=P(J)+ZINTP(K+1)*C(NCI+1,K+1)	MAIN455)
457: NCI=NCI+1 MAIN457C 458: IF(NCI.GT.NY) CO TO 2C MAIN4580 459: GO TC 100C MAIN459C 460: C MAIN460C 461: C PRINT AND STORE THE RESULTS MAIN4610 462: C MAIN4620 463: 12 CONTINUE MAIN4630 464: IOK YP=0 MAIN4640 465: IOKYM=0 MAIN4650 466: C10Y=D1Y MAIN4662 467: D20Y=D2Y MAIN467C	456:	42	CONTINUE	MAIN456C
458: IF(NCI.GT.NY) GO TO 20 MAIN4580 459: GO TO 1000 MAIN4590 460: C MAIN4600 461: C PRINT AND STORE THE RESULTS MAIN4610 462: C MAIN4620 MAIN4620 463: 12 CONTINUE MAIN4630 MAIN4630 464: IOK YP=0 MAIN4640 MAIN4640 465: IOK YM=0 MAIN4650 MAIN4650 466: D10Y=D1Y MAIN4660 MAIN4660 467: D20Y=D2Y MAIN4670	457:		NCI=NCI+1	MAIN457C
459: GO TC 100C MAIN459C 460: C MAIN460C 461: C PRINT AND STORE THE RESULTS MAIN4610 462: C MAIN4620 MAIN4620 463: 12 CONTINUE MAIN4630 MAIN4630 464: IOK YP=0 MAIN4640 MAIN4640 465: IOK YM=0 MAIN4650 MAIN4650 466: C1 0Y=D1Y MAIN466C MAIN466C 467: D20Y=D2Y MAIN4670	458:		IF(NCI.GT.NY) CO TO 20	MAIN4580
460: C MAIN4600 461: C PRINT AND STORE THE RESULTS MAIN4610 462: C MAIN4620 463: 12 CONTINUE MAIN4630 464: IOK YP=0 MAIN4640 465: IOK YM=0 MAIN4650 466: D10Y=D1Y MAIN4660 467: D20Y=D2Y MAIN4670	459:		GO TC 100C	MAIN459C
461: C PRINT AND STORE THE RESULTS MAIN4610 462: C MAIN4620 463: 12 CONTINUE MAIN4630 464: IOKYP=0 MAIN4640 465: IOKYM=0 MAIN4650 466: PIOY=DIY MAIN4660 467: D20Y=D2Y MAIN4670	460:	С		MAIN4600
462: C MAIN4620 463: 12 CONTINUE MAIN4630 464: IOKYP=0 MAIN4640 465: IOKYM=0 MAIN4650 466: D10Y=D1Y MAIN4660 467: D20Y=D2Y MAIN4670	461:	С	PRINT AND STORE THE RESULTS	MAIN4610
463: 12 CONTINUE MAIN4630 464: IOKYP=0 MAIN4640 465: IOKYM=0 MAIN4650 466: D10Y=D1Y MAIN4660 467: D20Y=D2Y MAIN4670	462:	С		MAIN4620
464: IOKYP=0 MAIN4640 465: IOKYM=0 MAIN4650 466: DIOY=DIY MAIN4660 467: D20Y=D2Y MAIN4670	463:	12	CONTINUE	MAIN4630
465: IOKYM=0 NAIN4650 466: D10Y=D1Y MAIN4660 467: D20Y=D2Y MAIN4670	464:		I OK YP=0	MAIN4640
466: D10Y=D1Y MAIN4660 467: D20Y=D2Y MAIN4670	465:		IOKYM=0	MAIN4650
467: D20Y=D2Y MAIN4670	466:		C17Y=D1Y	MAIN4662
	467:		D 2 Q Y = D 2 Y	MAIN4670

468:		D17Z=D1Z	MAIN4680
469:		D2CZ=D2Z	MAIN4690
470:		CO 66 I=1,NTY	MAIN4710
471:		EHCO(I)=1000.D9*EHCO(I)	MAIN4710
472:		CO 66 J=1,NTZ	MAIN4720
473:		IF(I.FQ.1) CECO(J)=CECO(J)*1000.DC	MAIN4730
474:		$IF(I \bullet EQ \bullet 1) CECCY(J) = CECOY(J) * 1000 \bullet D0$	MAIN474C
475:		CC(I,J) = C(I,J)	MAIN475C
476:	66	C(I,J)=C(I,J)*16CŮ.D0	MAIN4760
477:		CC01=1000.C0*CC01	MAIN4770
478:		CCN3=1000.DA*CCD3	MAIN4780
479:		WRITE(6,5CC) ACTX,Q,IHLF	MAIN4791
48.7:	5 าก	FURMAT(2(/),2CX,'X =',F12.3,20X,'Q =',F1C.2,10X,'IHLF =',I5,/)	MAIN48CD
481:		WRITE(6,200)	MAIN4813
482:	2000	FORMAT(2(/))	MAIN4823
483:		WRITE(6,352) (ACTY(I), $I=1$, NTYH), ARYC	MAIN483J
484:	352	FORMAT(1X,132(***)/1X,** Z/Y **,1CF12.2,* **)	MAIN484C
485:		WRITE(6,65°)	MAIN485C
486:	58	CONTINUE	MAIN4867
487:		I=NTZ	MAIN4870
488:	572	CONTINUE	MAIN488C
489:		WRITE(6,3CC) ACTZ(I),(C(J,I),J=1,NTYH),CECC(I)	MAIN489J
470:	30n	FORMAT(1X, ***, F7.2, 1X, ***, 10F12.5, * **)	MAIN49C)
491:		I = I - 1	MAIN491C
492:		IF(I.EQ.C) GO TO 501	MAIN4920
473:		GO TO 502	MAIN4937
494:	501	CONTINUE	MAIN4943
495:		WRITE(6,65C)	MAIN4950
496:	650	FCRMAT(1X,132(***))	MAIN4960
497:		WPITE(6,3C0) HSEL,(EHCC(I),I=1,NTYH),CCO1	MAIN497C
498:		WRITE(6,200)	MAIN4980
499:		WRITE(6,352) (ACTY(I),I=NTYH1,NTY),ARYC	MAIN4990
530:		WPITE(6,650)	MAINSCOJ
561:	608	CONTINUE	MAIN5010
5]2:		I=NTZ	MAIN5020
503:	55+2	CUNTINUE	MAIN5030

			PAGE 15
504:		<pre>write(6,3cc) actz(I),(C(J,I),J=ntyH1,nty),Cecoy(I)</pre>	MAIN5040
505:		I = I - 1	MAIN5750
566:		IF(I.EQ.U) GD TO 5501	MAIN5060
507:		GO TO 5502	MAIN5C70
508:	5501	CONTINUE	MAIN5787
509:		hRITE(6,65C)	MAIN5090
510:		WRITE(6,3CC) HSEL,(EHCC(I),I=NTYH1,NTY),CCC3	MAIN5100
511:		IF(IST.EQ.1) STOP	MAIN5110
512:		GO TC 1	MAIN512C
513:	910	CONTINUE	MAIN513C
514:		END	MAIN5147

1: 2:	C	SUBROUT INE	DRKGS(PRMT,Y,DERY,NDIM,IHLF,FCT,AUX,PW)	DRKG DRKG	1) 20
3:	C C	THIC CHODOUTS	NE COLVES & SYSTEM OF EIDST OPDED OPDIANDY DIFFEDENTIAL		5U A O
4. 5.	c c	ECHATIONS WIT	NE SUEVES A STSTEM OF FIRST URDER URDINART DIFFERENTIAL.		- 4 -9 - 61
- J •	ĉ	TCCATIONS WIT	H GIVEN INITIAL CONDITIONS	TPKC	60
7.	r r			CRKC	7.1
8.	r r	DPMT	- AN INDUT OUTPUT VECTOR WITH CIMENSION GREATER OR	DRKG	80
9:	č	1 EV.) > 1	ECHAL TO 5	CKKG	90
10:	č	PRMT(1)	- LOWER BOUND OF THE INTERVAL	CRKG	100
11:	č	PRMT(2)	- UPPER BOUND OF THE INTERVAL	CRKG	110
12:	Č	PRMT(3)	- INITIAL INCREMENT OF THE INCEPENDENT VARIABLE	DRKG	120
13:	С	PRMT(4)	- UPPER ERRCP BOUND	CRKG	130
14:	С	PRMT(5)	- NO INPUT PARAMETER. IT IS C UNLESS THE USER WANTS TO	CRKG	140
15:	С		TERMINATE RKGS AT ANY OUTPUT POINT	CRKG	150
16:	С	DERY	- INPUT VECTOR OF ERROR WEIGHTS. LATERON IS THE VECTOR	DRKG	160
17:	С		OF DERIVATIVES	CRKG	170
18:	С	NCIM	- THE NUMBER OF EQUATIONS IN THE SYSTEM	CRKG	180
19:	C	IHLF	- THE NUMBER OF BISECTIONS OF THE INITIAL INCREMENT	DRKG	190
20:	С	AUX	- AN AUXILIARY STORAGE ARRAY (8 REWS AND NDIM COLUMNS)	CRKG	200
21:	C			DRKG	210
22:	C			DRKG	220
23:		IMPLICIT R	EAL*8(A-H,G-Z)	LKKG	230
24:			Y(1), UERY(1), AUX(8, 1), A(4), B(4), U(4), PRMI(1),		24 J
25:		LPWINUIM,NL			256
20.		1 1 1 = 1 1 1 = 1 1 1 = 1 1			200
21.		1 AUA(0,17-L Y-00MT/1)		DRKC	280
20.			21	DRKC	200
30:		H=DRMT(3)		DRKG	300
31:		PRMT(5)=0	ro.	CRKG	310
32:		CALL ECT (Y	NCIM-DERY-PW)	CRKG	320
33:	С			CRKG	330
34:	Ċ	FRRCR TEST		CRKG	340
35:	С			DRKG	35C

36: IF(H*(XENE-X))36,37,2 DRKG 360 37: C DRKG 37C 38: C PREPARATIONS FOR RUNGE-KUTTA METHED DRKG 390 39: C C CRKG 391 40: 2 A(1)=.5D) DRKG 400 DRKG 410 41: A(2)=.29289321881345248D0 DRKG 420 DRKG 420 42: A(3)=1.7071067811865475DC DRKG 420 DRKG 420 43: A(4)=.1666666666666666666666666666666666666	2
36: IF(H*(XENL-X))36,37,2 DRkG 360 37: C DRkG 37C 38: C PREPARATIONS FOR RUNGE-KUTTA METHED DRkG 37C 39: C C ERKG 380 40: 2 A(1)=.5D) DRkG 400 ERKG 41C 41: A(2)=.29289321881345248D0 DRkG 41C DRkG 420 42: A(3)=1.7071067811865475DC DRkG 430 DRkG 430 43: A(4)=.1666666666666666666666666666666666666	
37: C DRKG 37G 38: C PREPARATIONS FOR RUNGE-KUTTA METHED DRKG 380 39: C ERKG 390 ERKG 390 40: 2 A(1) = •5D) DRKG 40° ERKG 410 41: A(2) = •29289321881345248D0 ERKG 410 ERKG 420 42: A(3) = 1 • 7071067811865475DC ERKG 420 ERKG 430 43: A(4) = •166666666666666666666666666666666666	
38: C PREPARATIONS FOR REINGE-RETTA METHED CRKG 380 39: C C CRKG 390 40: 2 A(1)=.5D) DRKG 40° 41: A(2)=.29289321881345248D0 CRKG 410 42: A(3)=1.7071067811865475DC CRKG 420 43: A(4)=.1666666666666666666666666666666666666	
39: C CRKG 390 40: 2 A(1)=.5D) CRKG 40° 41: A(2)=.29289321881345248D0 CRKG 410 42: A(3)=1.7071067811865475DC CRKG 420 43: A(4)=.1666666666666666666666666666666666666	
40: $2 A(1) = .50$ DRKG 40°41: $A(2) = .2928932188134524800$ ERKG 41042: $A(3) = 1.707106781186547500$ ERKG 42043: $A(4) = .166666666666666666666666666666666666$	
41: A(2) = .29289321881345248D0 CRKG 410 42: A(3) = 1.7071067811865475D0 CRKG 420 43: A(4) = .166666666666666666666666666666666666	
42: $A(3) = 1.70710678118654750C$ CRKG 42043: $A(4) = .166666666666666670C$ CRKG 43044: $B(1) = 2.0J$ CRKG 44045: $E(2) = 1.0C$ CRKG 45046: $B(3) = 1.CC$ CRKG 46047: $B(4) = 2.0^{11}$ CRKG 47043: $C(1) = .5DC$ CRKG 48049: $C(2) = .29289321881345248DC$ CRKG 49050: $C(3) = 1.7071067811865475D^{0}$ CRKG 500	
43: $A(4) = .16666666666666666700$ CRKG 43044: $B(1) = 2.0J$ CRKG 44045: $E(2) = 1.00$ CRKG 45046: $B(3) = 1.00$ CRKG 46047: $B(4) = 2.0^{11}$ CRKG 47043: $C(1) = .500$ CRKG 48049: $C(2) = .2928932188134524800$ CRKG 49050: $C(3) = 1.70719678118654750^{10}$ CRKG 500	
44: B(1)=2.DJ DRKG 440 45: B(2)=1.DG DRKG 450 46: B(3)=1.CC DRKG 460 47: B(4)=2.D% DRKG 470 43: C(1)=.5DC DRKG 480 49: C(2)=.29289321881345248DC DRKG 490 50: C(3)=1.7071067811865475D0 DRKG 5CC	
45: E(2)=1.D0 ERKG 450 46: B(3)=1.C0 DRKG 460 47: B(4)=2.D4 DRKG 470 43: C(1)=.5DC DRKG 480 49: C(2)=.29289321881345248DC DRKG 490 50: C(3)=1.7071067811865475D0 DRKG 500	
46: B(3)=1.CC DRKG 460 47: B(4)=2.D ⁽¹⁾ DRKG 470 43: C(1)=.5DC DRKG 480 49: C(2)=.29289321881345248DC DRKG 490 50: C(3)=1.7071067811865475D0 DRKG 500	
47: B(4)=2.04 DRKG 470 43: C(1)=.5DC DRKG 487 49: C(2)=.29289321881345248DC DRKG 490 50: C(3)=1.7071967811865475D0 DRKG 500	
43: C(1)=.5DC DRKG 481 49: C(2)=.29289321881345248DC DRKG 490 50: C(3)=1.7071967811865475D0 DRKG 500	
49: C(2)=.29289321881345248DC CRKG 490 50: C(3)=1.7071967811865475D0 CRKG 5CC	
50: C(3)=1.7071067811865475D0 CRKG 5CC	
51: U(4)=•50C ERKG 510	
52: C ERKG 520	
53: C PREPARATIONS OF FIRST RUNGE-KUTTA STEP DRKG 53J	
54: C DRKG 540	
55: DO 3 I=1,NDIM CRKG 550	
56: $AUX(1,I)=Y(I)$ DRKG 56)	
57: AUX(2,I)=CERY(I) DRKG 570	
58: AUX(3,I)=C.DC CRKG 58C	
59: 3 AUX(6,I)=C.Dn CRKG 59)	
60: IREC=0 DRKG 600	
61: H=H+H CRKG 610	
62: IHLF=-1 CRKG 620	
63: ISTEP=7 CRKG 630	
64: IEND= 2 DRKG 640	
65: C	
66: C STAPT OF A RUNGE-KUTTA STEP CRKG 660	
67: C	
68: 4 IF((X+H→XEND)*H)7.6.5 CRKG 683	
69: 5 H=XENC-X	
7): 6 [END=1 DRKG 706	
71: C	

72: C C C DRKG 72C 73: C C CRKG 73C 74: 7 CONTINUE CRKG 73C 75: 1F(PRMT(5))49,8,4.) CKKG 75C 76: 7: 9 ISTEP=ISTEP+1 CRKG 77C 78: C CRKG 75C 79: C START OF INNERMOST RUNGE-KUTTA LCCP CRKG 75C 70: C START OF INNERMOST RUNGE-KUTTA LCCP CRKG 75C 70: C J=1 CRKG 75C 71: J=1 CRKG 75C CRKG 75C 71: J=1 CRKG 75C CRKG 75C 72: C START OF INNERMOST RUNGE-KUTTA LCCP CRKG 75C 71: J=1 CRKG 75C CRKG 75C 72: C J=2 CLJ CRKG 75C 73: J=1 CRKG 82C CRKG 82C 74: Y AJ=A(J) CRKG 842 CRKG 842 75: D0 11 I=1,N01M CRKG 842 CRKG 842 76: R2=24R2+R2 CRKG 842 CRKG 842 77: R2=AJ*(R1+6J*AUX(6,1)+R2-CJ*R1 CRKG 922 CRKG 922 77: I AUX(6,1)=ALX(6,1)+R2-CJ*R1 CRKG 922 CRKG 922 77: I F(J-3)13,14,13 CRKG 922 CRKG 922 77: I F(J-3)13,14				
73: C CRNTINUE CRKC 740 74: 7 CONTINUE CRKC 740 75: IF(PRMT(5))40,8,4.) CRKC 75C 76: 9 ISTCP=ISTEP+1 CRKC 77C 79: C START OF INNERMOST RUNGE-KUTTA LCCP CRKG 76C 79: C START OF INNERMOST RUNGE-KUTTA LCCP CRKG 76C 79: C START OF INNERMOST RUNGE-KUTTA LCCP CRKG 800 81: J=1 CRKG 810 CRKG 820 82: 1' AJ=A(J) CRKG 820 CRKG 820 84: CJ=C(J) CRKG 820 CRKG 820 85: D0 11 I=1,NDIM CRKG 820 CRKG 820 86: R1=H#DERV(1) CRKG 820 CRKG 820 87: Y(1)=Y(1)+82 CRKG 820 CRKG 820 98: Y(1)=Y(1)+82 CRKG 820 CRKG 820 91: IF(J-4)12,15,15 CRKG 820 CRKG 820 91: IF(J-4)12,15,15 CRKG 920 CRKG 920 91: IF(J-4)12,15,15 CRKG 920 CRKG 920 92: I2 J=J=H CRKG 920 CRKG 920 <td< td=""><td>72:</td><td>С</td><td>RECORDING OF INITIAL VALUES OF THIS STEP</td><td>DRKG 72C</td></td<>	72:	С	RECORDING OF INITIAL VALUES OF THIS STEP	DRKG 72C
74: 7 CONTINUE CRKG 76C 75: IFEPRT(5))40,8,4.) CRKG 75C 76: 9 ITEST=0 CRKG 76C 77: 9 ISTEP=ISTEP+1 CRKG 76C 78: C CRKG 76C 79: C START OF INNERMOST RUNGE=KUTTA LCCP CRKG 76C 79: C START OF INNERMOST RUNGE=KUTTA LCCP CRKG 810 82: I* AJ=A(J) CRKG 82C CRKG 82C 81: J=1 CRKG 83C CRKG 82C 82: I* AJ=A(J) CRKG 82C CRKG 83C 85: CD 11 I=1,NDIM CRKG 84C CRKG 84C 85: CD 11 I=1,NDIM CRKG 82C CRKG 84C 86: R1=HDERY(I) CRKG 84C CRKG 84C 87: Y(I)=Y(I)+82 CRKG 84C CRKG 84C 93: If (J=4)12,15,15 CRKG 84C CRKG 940 91: IF(J=4)13,14,13 CRKG 940 CRKG 940 92: 12 J=J1 CRKG 85C CRKG 95C 93: IF (J=2)13,14,13 CRKG 96C CRKG 97C 94: IX SX+SD2++ CRKG 97C	73:	С		ERKG 730
75: IF(PRPT(5))40,8,4) CKG 75C 76: 9 ISTEP=ISTEP+1 CRKG 76C 77: 9 ISTEP=ISTEP+1 CRKG 77C 78: C CRKG 76C 79: C CRKG 76C 79: C CRKG 76C 79: C CRKG 76C 79: C CRKG 76C 81: J=1 CRKG 82C 82: I' AJ=A(J) CRKG 82C 83: GJ=R(J) CRKG 82C 84: CJ=C(J) CRKG 82C 85: CO II I=1,NDIM CRKG 82C 84: CJ=C(J) CRKG 82C 85: R2=AJ*(R1-BJ*AUX(6,I)) CRKG 82C 86: R1=H*DERY(I) CRKG 82C 87: R2=AJ*(R1-BJ*AUX(6,I)) CRKG 82C 93: II AUX(6,I)=ALX(6,I)+R2=CJ*R1 CRKG 87C 94: Y(I)=Y(I)+R2 CJ*RI 95: R2=AJ*(R2+R2 CRKG 89C 91: IF(I-J)12,15,15 CRKG 910 92: I2 J=J+1 CRKG 92C 93: IF(J=A)112,14,13 CRKG 92C <	74:		7 CONTINUE	ERKG 740
76: 9 ITEST=0 CPKG 76C 77: 9 ISTEP=ISTEP+1 CPKG 77C 78: C CPKG 77C 79: C START OF INNERMEST RUNGE-KUTTA LCCP CPKG 78C 79: C START OF INNERMEST RUNGE-KUTTA LCCP CPKG 78C 79: C START OF INNERMEST RUNGE-KUTTA LCCP CPKG 78C 70: J=1 CPKG 78C CPKG 800 81: J=1 CPKG 82C CPKG 82C 81: J=1 CPKG 82C CPKG 82C 82: HJ=K(J) CPKG 82C CPKG 82C 84: CJ=C(J) CPKG 82C CPKG 82C 85: D0 11 I=1,NDIM CPKG 82C CPKG 82C 86: R1=H+DERY(I) CPKG 82C CPKG 82C 87: R2=AJ*(R1-BJ*AUX(6,1)) CPKG 82C CPKG 82C 87: R2=AJ*(R1-BJ*AUX(6,1)+R2=CJ*R1 CPKG 82C CPKG 82C 91: IF(J-4)12,16,15 CPKG 920 CPKG 82C 91: IF(J-4)12,16,15 CPKG 92C CPKG 92C 91: IF(J-4)12,16,15 CPKG 92C CPKG 92C 92: Iz J=J+1 <t< td=""><td>75:</td><td></td><td>IF(PRMT(5))49,8,40</td><td>DRKG 75C</td></t<>	75:		IF(PRMT(5))49,8,40	DRKG 75C
77: 9 ISTEP=ISTEP+1 CPKG 770 78: C CPKG 770 79: C START OF INNERMOST RUNGE-KUTTA LCCP CPKG 780 80: J=1 CPKG 780 81: J=1 CPKG 780 82: I^AJ=A(J) CPKG 800 83: BJ=R(J) CPKG 820 84: CJ=C(J) CPKG 840 85: D0 11 I=1,NDIM CPKG 840 86: R1=H*DERV(I) CPKG 870 87: R2=AJ*(R1=BJ*AUX(6,I)) CPKG 870 98: Y(I)=Y(1)+82 CPKG 820 89: R2=A2+R2+R2 CPKG 870 91: IF(J-4)12,15,15 CPKG 920 91: IF(J-4)12,15,15 CPKG 920 91: IF(J-4)12,15,15 CPKG 920 92: 12 J=J+1 CPKG 920 93: IF(J-3)13,14,13 CPKG 920 94: 13 X=X+,502*H CPKG 920 95: I4 CALL FCT(Y,NEIM,DERY,PW) CPKG 920 96: GOTO 10 CPKG 920 97: C CPKG 920 97: C	76:		8 ITEST=0	DRKG 76C
78: C C CFKG 78C 79: C START OF INNERMOST RUNGE-KUTTA LCCP DRKG 78C 80: C CRKG 800 DRKG 820 81: J=1 DRKG 820 DRKG 820 82: HJ=R(J) DRKG 820 DRKG 820 84: CJ=C(J) DRKG 820 DRKG 820 85: D0 11 I=1,NDIM DRKG 820 DRKG 820 86: R1=H#DERY(I) DRKG 820 DRKG 820 87: R2=AJ*(R1=BJ*AUX(6,I)) DRKG 820 DRKG 820 93: Y(I)=Y(I)+R2 DRKG 820 DRKG 820 93: IF(J=4)12,15,15 DRKG 920 DRKG 920 93: IF(J=4)12,15,15 DRKG 920 DRKG 920 93: IF(J=3)13,14,13 DRKG 920 DRKG 920 94: I 2 J=J1 DRKG 920 DRKG 920 95: I 4 CALL FCT(Y,NDIM,DERY,PW) DRKG 920 DRKG 920 95: I 4 CALL FCT(Y,NDIM,DERY,PW) DRKG 920 DRKG 920 97: C GR DRKG 930 DRKG 930 97: C IF(I=EST)16,16,20 DRKG 930 DRKG 930 97: C IF(I TEST)16,16,20 DRKG 930 DRKG 930 10: C IF(I TEST)16,16,20 DRKG 930 </td <td>77:</td> <td></td> <td>9 ISTEP=ISTEP+1</td> <td>ERKG 770</td>	77:		9 ISTEP=ISTEP+1	ERKG 770
79: C START OF INNERMOST RUNGE-KUTTA LCCP DRKG 79C 80: C DERKG 800 DRKG 810 81: J=1 DRKG 810 DRKG 820 82: I' AJ=A(J) DRKG 820 RKG 840 83: HJ=R(J) DRKG 840 DRKG 840 84: CJ=C(J) DRKG 840 DRKG 840 85: D0 11 I=1,NDIM DRKG 850 DRKG 860 86: R1=H+DERY(I) DRKG 860 DRKG 860 87: R2=AJ+(R1=BJ*AUX(6,I)) DRKG 860 DRKG 860 97: Y(I)=Y(I)+R2 DRKG 880 DRKG 890 93: I1 AUX(6,I)=AUX(6,I)+R2-CJ*R1 DRKG 890 DRKG 890 91: IF(J-4)12,15,15 DRKG 910 DRKG 920 92: I2 J=J+1 DRKG 920 IF(G 930 93: IF(J-3)13,14,13 DRKG 920 RKG 940 94: I3 X=X+500*H DRKG 920 DRKG 920 95: I4 CALL FCT(Y,NDIM,DERY,PW) DRKG 920 DRKG 920 96: C TEST OF ACCURACY DRKG 930 97: C GR DRKG 930 97: C TEST OF ACCURACY DRKG 930 97: C IF(ITEST)16,16,20 DRKG 930 10: C DRKG192 <td>78:</td> <td>С</td> <td></td> <td>DRKG 780</td>	78:	С		DRKG 780
80: C CRKG 800 81: J=1 CRKG 810 82: 17 AJ=A(J) DRKG 820 83: HJ=R(J) CRKG 830 84: CJ=C(J) CRKG 850 85: D0 11 I=1,NDIM CRKG 850 86: R1=H*DERY(I) CRKG 850 87: R2=AJ*K(R1=BJ*AUX(6,I)) CRKG 860 87: R2=AJ*K(R1=BJ*AUX(6,I)) CRKG 860 87: R2=AJ*K(R1=BJ*AUX(6,I)+R2=CJ*R1 CRKG 870 90: 14 AUX(6,I)=AUX(6,I)+R2=CJ*R1 CRKG 970 91: 1F(J=4)12,15,15 CRKG 910 92: 12 J=J+1 CRKG 920 93: IF(J=3)13,14,13 CRKG 920 94: 13 X=X+.502*F CRKG 920 95: I4 CALL FCT(Y,NDIM,DERY,PW) CRKG 920 97: C CRKG 933 97: C CRKG 930 10: C CRKG 930 <	79:	С	START OF INNERMOST RUNGE-KUTTA LOOP	DRKG 79C
81: J=1 DRKG 810 82: 1 ^r AJ=A(J) DRKG 823 83: BJ=R(J) DRKG 823 84: CJ=C(J) DRKG 847 85: DO 11 I=1,NDIM DRKG 850 86: R1=H#DERY(I) DRKG 850 87: R2=AJ*(R1-BJ*AUX(5,I)) DRKG 860 98: Y(1)=Y(1)+82 DRKG 870 99: I1 AUX(6,I)=AUX(6,I)+R2=CJ*R1 DRKG 970 91: IF(J-4)12,15,15 DRKG 920 92: I2 J=J+1 DRKG 920 93: IF(J-3)13,14,13 DRKG 920 94: I3 X=X+,5D0*+ DRKG 920 95: I4 CALL FCT(Y,NDIM,DERY,PW) DRKG 920 97: C DRKG 950 97: C DRKG 960 97: C DRKG 970 97: C DRKG 970 97: C DRKG 980 97: <	8 0:	С		ERKG 800
82: 1 ^r AJ=A(J) DRKG 820 83: HJ=R(J) DRKG 840 84: CJ=C(J) DRKG 840 85: DO 11 I=1,NDIM DRKG 850 86: R1=H#DERY(I) DRKG 860 87: R2=AJ#(R1=BJ#AUX(6,I)) DRKG 870 97: Y(I)=Y(I)+82 DRKG 870 89: R2=324R2+R2 DRKG 870 90: I1 AUX(6,I)=AUX(6,I)+R2=CJ#R1 DRKG 970 91: IF(J=4)12,15,15 DRKG 920 92: 12 J=J+1 DRKG 920 93: IF(J=3)13,14,13 DRKG 920 94: 13 X=x+,5DD#+ DRKG 921 95: 14 CALL FCT(Y,NDIM, DERY, PW) DRKG 930 96: G TEST OF ACCURACY DRKG 933 97: C DRKG 933 97: C DRKG 930 97: C DRKG 930 97: C DRKG 933 97: C DRKG 933 97: C DRKG 933 97: C DRKG 920 10: IF(ITEST)16,16,20 DRKG 920	81:		J=1	CRKG 810
83: BJ=R(J) CRKG 83^ 84: CJ=C(J) CRKG 840 85: DO 11 I=1,NDIM CRKG 850 86: R1=H=DERY(I) CRKG 850 87: R2=AJ#(R1=BJ*AUX(6,I)) CRKG 870 98: Y(I)=Y(I)+82 CRKG 870 99: R2=R2+R2+R2 CRKG 970 90: If AUX(6,I)=AUX(6,I)+R2=CJ*R1 CRKG 970 91: IF(J=4)12,15,15 CRKG 920 92: 12 J=J+1 CRKG 920 93: IF(J=3)13,14,13 CRKG 930 94: 13 X=X+.5D0*F CRKG 940 95: 14 CALL FCT(Y,NDIM, DERY, FW) CRKG 960 97: GOTO 10 CRKG 960 97: C CEST OF ACCURACY DRKG 930 97: C IF(ITEST)16,16,20 CRKG 970 10: C CRKG 970 CRKG 970 10: 15 IF(ITEST)16,16,20 CRKG 970 CRKG1020 10: C C CRKG1020 CRKG1020 10: C C CRKG1020 CRKG1020 10: C <t< td=""><td>82:</td><td></td><td>$1^{\prime} \Delta J = \Delta (J)$</td><td>DRKG 820</td></t<>	82:		$1^{\prime} \Delta J = \Delta (J)$	DRKG 820
84: CJ=C(J) CRKG 840 85: DO 11 I=1,NDIM CRKG 850 86: R1=H*DERY(I) CRKG 860 87: R2=AJ*(R1=BJ*AUX(5,I)) CRKG 860 98: Y(I)=Y(I)+R2 CRKG 860 89: R2=32+R2+R2 CRKG 890 90: I1 AUX(6,I)=ALX(6,I)+R2=CJ*R1 CRKG 970 91: IF(J-4)12,15,15 CRKG 920 92: 12 J=J+1 CRKG 920 93: IF(J-3)13,14,13 CRKG 920 94: 13 X=X+,5D0*H CRKG 940 95: I4 CALL FCT(Y,NDIM,DERY,PW) CRKG 960 96: GOTO 10 CRKG 960 97: C CRKG 970 98: C TEST OF ACCURACY CRKG 970 99: C TEST OF ACCURACY CRKG 970 100: 15 IF(ITEST)16,16,20 CRKG 970 101: C CRKG 100 102: C IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING CF ACCURACY CRKG1020 103: C CRKG1020 CRKG1020 104: IF <st=1< td=""> CRKG1020 CRKG1020 <</st=1<>	83:		BJ=B(J)	CRKG 830
85: DO 11 I=1,NDIM DRKG 25C 86: R1=H*DERY(I) DRKG 86C 87: R2=AJ*(R1=BJ*AUX(6,I)) DRKG 86C 87: R2=AJ*(R1=BJ*AUX(6,I)) DRKG 870 98: Y(I)=Y(I)+R2 DRKG 88C 89: R2=R2+R2+R2 DRKG 970 91: I AUX(6,I)=AUX(6,I)+R2=CJ*R1 DRKG 970 91: IF(J-4)12,15,15 DRKG 920 92: 12 J=J+1 DRKG 920 93: IF(J-3)13,14,13 DRKG 920 94: 13 X=X+,5D2*F DRKG 940 95: I 4 CALL FCT(Y,NDIM,DERY,PW) DRKG 930 96: GFT 0 DRKG 930 97: C DRKG 930 98: C TEST OF ACCURACY DRKG 930 99: C IS IF(ITEST)16,16,20 DRKG 930 10: 15 IF(ITEST)16,16,20 DRKG 920 DRKG 930 10: C IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING CF ACCURACY DRKG102C 10: C IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING CF ACCURACY DRKG102C 10: I 5 ED0 17 I=1,NDIM DRKG102C	84:		CJ = C(J)	CRKG 840
86: R1=H*DERY(I) CRKG 66C 87: R2=AJ*(R1=BJ*AUX(6,I)) CRKG 670 98: Y(I)=Y(I)+R2 CRKG 870 99: R2=32+R2+R2 CRKG 870 90: 11 AUX(6,I)=AUX(6,I)+R2-CJ*R1 CRKG 910 91: IF(J-4)12,15,15 CRKG 910 92: 12 J=J+1 CRKG 920 93: IF(J-3)13,14,13 CRKG 930 94: 13 X=X+500*+ CRKG 940 95: 14 CALL FCT(Y,NDIM,DERY,PW) CRKG 96C 97: C CRKG 930 97: C CRKG 930 97: C CRKG 96C 97: C CRKG 96C 97: C CRKG 96C 97: C CRKG 970 97: C CRKG 970 97: C CRKG 96C 13 X=X+5C0*+ CRKG 96C CRKG 96C 130: 15 IF(ITEST)16,16,20 CRKG 96C 130: 15 IF(ITEST)16,16,20 CRKG102C 14: 16 D0 17 I=1,NDIM CRKG102C 14: 16 D0 17 I=1,NDIM	85:		DO 11 I=1, NDIM	DRKG 850
87: R2=AJ*(R1-BJ*AUX(6,I)) CRKG 870 98: Y(I)=Y(I)+R2 CRKG 880 89: R2=R2+R2+R2 CRKG 870 90: 11 AUX(6,I)=ALX(6,I)+R2-CJ*R1 CRKG 910 91: IF(J-4)12,15,15 CRKG 910 92: 12 J=J+1 CRKG 920 93: IF(J-3)13,14,13 CRKG 940 94: 13 X=X+.5C0*F CRKG 940 95: I4 CALL FCT(Y,NDIM,DERY,PW) CRKG 960 96: GOTO 10 CRKG 960 97: C CRKG 970 98: C TEST OF ACCURACY DRKG 960 99: C IF(ITEST)16,16,20 CRKG 970 101: C CRKG 970 CRKG 970 102: C IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING CF ACCURACY CRKG1020 103: C CRKG1020 CRKG1020 CRKG1020 104: 16 D0 17 I=1,NDIM CRKG1020 CRKG1020 104: 16 D0 17 I=1,NDIM CRKG1020 CRKG1020 105: 17 MUX(4,I)=Y(I) CRKG1020 CRKG1020 106: ITEST=1	:63		R1=H*DERY(I)	CRKG 86C
98: Y(I)=Y(I)+R2 CRKG 88C 89: R2=R2+R2+R2 CRKG 89C 90: 11 AUX(6,I)=AUX(6,I)+R2=CJ*R1 CRKG 910 91: IF(J=4)12,15,15 CRKG 910 92: 12 J=J+1 CRKG 920 93: IF(J=3)13,14,13 CRKG 940 94: 13 X=X+.5D0*H CRKG 940 95: 14 CALL FCT(Y,NDIM,DERY,PW) CRKG 960 96: GOTO 10 CRKG 960 97: C CRKG 970 98: C TEST OF ACCURACY CRKG 933 99: C ISTEPTION THERE IS NO POSSIBILITY FOR TESTING CF ACCURACY CRKG1020 101: C CRKG1020 CRKG1020 CRKG1020 102: C IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING CF ACCURACY CRKG1020 104: 14 CD 17 I=1,NDIM CRKG1020 CRKG1020 104: 14 CD 17 I=1,NDIM CRKG1020 CRKG1020 105: 17 AUX(4,I)=Y(I) CRKG1020 CRKG1020 105: ITEST=1 CRKG1020 CRKG1020 106: ITEST=1 CRKG1020 CRKG1020 <td>87:</td> <td></td> <td>R2=AJ*(R1-BJ*AUX(6,I))</td> <td>ERKG 870</td>	87:		R2=AJ*(R1-BJ*AUX(6,I))	ERKG 870
89: R2=R2+R2+R2 CRKG P3C 90: 11 AUX(6,I)=ALX(6,I)+R2=CJ*R1 CRKG 930 91: IF(J=4)12,15,15 CRKG 92C 92: 12 J=J+1 CRKG 937 93: IF(J=3)13,14,13 CRKG 937 94: 13 x=X+,5C0*+ CRKG 941 95: 14 CALL FCT(Y,NDIM,DERY,PW) CRKG 96C 97: C CRKG 973 98: C TEST OF ACCURACY DRKG 933 99: C CRKG 99C 100: 15 IF(ITEST)16,16,20 CRKG 99C 101: C CRKG 102C 102: C IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING CF ACCURACY CRKG102C 103: C C CRKG102C 104: 16 D0 17 I=1,NDIM CRKG102C CRKG1032 104: 16 D0 17 I=1,NDIM CRKC1040 CRKG1051 105: 17 AUX(4,I)=Y(I) CRKG1051 CRKG1051 105: IT_EST=1 CRKG1020 CRKG1020 106: IT_EST=1 CRKG1020 CRKG1020	88:		Y(I) = Y(I) + R2	CRKG 880
9): 11 AUX(6,I)=AUX(6,I)+R2-CJ*R1 CRKG 900 91: IF(J-4)12,15,15 CRKG 910 92: 12 J=J+1 CRKG 920 93: IF(J-3)13,14,13 CRKG 930 94: 13 X=X+.5C0*F CRKG 940 95: 14 CALL FCT(Y,NDIM,DERY,PW) CRKG 960 96: GOTO 10 CRKG 960 97: C CRKG 970 98: C TEST OF ACCURACY DRKG 960 97: C CRKG 970 98: C TEST OF ACCURACY DRKG 930 97: C CRKG 960 97: C CRKG 970 98: C TEST OF ACCURACY DRKG 960 97: C CRKG 970 98: C TEST OF ACCURACY DRKG 930 97: C CRKG 100 101: C CRKG 100 11: C CRKG 100 12: C IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING CF ACCURACY CRKG1020 104: 16 D0 17 I=1,NDIM CRKC1040 105: 17 AUX(4,I)=Y(I) CRKG1050 104:	89:		R2=R2+R2+R2	DRKG 890
91: IF(J-4)12,15,15 DRKG 910 92: 12 J=J+1 DRKG 920 93: IF(J-3)13,14,13 DRKG 930 94: 13 X=X+.5D0*H DRKG 940 95: 14 CALL FCT(Y,NDIM,DERY,PW) DRKG 950 96: GOTO 10 DRKG 960 97: C DRKG 970 98: C TEST OF ACCURACY DRKG 960 97: C DRKG 960 98: C TEST OF ACCURACY DRKG 960 100: 15 IF(ITEST)16,16,20 DRKG 960 101: C DRKG 960 102: C IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING CF ACCURACY DRKG1020 104: 16 DO 17 I=1,NDIM DRKG1020 DRKG1020 104: 16 DO 17 I=1,NDIM DRKG1020 DRKG1020 105: 17 AUX(4,I)=Y(I) DRKG1020 DRKG1020 106: ITEST=1 DRKG1020 DRKG1020 107: ISTEP=1STEP+1STEP=2 DRK01070 DRKG1020	9):		11 AUX(6,I)=ALX(6,I)+R2-CJ*R1	CRKG 920
92: 12 J=J+1 DRKG 920 93: IF(J-3)13,14,13 CRKG 930 74: 13 X=X+.5D0*F CRKG 941 95: 14 CALL FCT(Y,NDIM,DERY,PW) CRKG 950 96: GOTO 10 CRKG 950 97: C CRKG 971 98: C TEST OF ACCURACY DRKG 930 99: C IF(ITEST)16,16,20 101: C CRKG1020 102: IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING CF ACCURACY DRKG1020 104: 16 DO 17 I=1,NDIM CRKG1020 105: 17 AUX(4,I)=Y(I) CRKG1051 106: ITEST=1 CRKG1051 107: ISTEP=ISTEP+ISTEP=2 CRKG1070	91:		IF(J-4)12,15,15	CRKG 910
93: IF(J-3)13,14,13 CRKC 930 94: 13 X=X+.5C0*F CRKG 941 95: 14 CALL FCT(Y,NDIM,DERY,PW) CRKG 550 96: GOTO 10 CRKG 960 97: C CRKG 970 98: C TEST OF ACCURACY DRKG 930 98: C TEST OF ACCURACY DRKG 930 98: C TEST OF ACCURACY DRKG 930 100: 15 IF(ITEST)16,16,20 CRKG100 101: C CRKG100 102: IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING CF ACCURACY CRKG1020 104: 16 D0 17 I=1,NDIM CRKC1040 105: I7 AUX(4,I)=Y(I) CRKG1050 106: ITEST=1 CRKG1020 107: LSTEP=1STEP+1STEP=2 CRKG1020	92:		12 J = J + 1	DRKG 920
74: 13 X=X+.5DD*H CRKG 941 95: 14 CALL FCT(Y,NDIM,DERY,PW) CRKG 550 56: GOTO 10 CRKG 962 97: C CRKG 963 98: C TEST OF ACCURACY CRKG 962 10: 15 IF(ITEST)16,16,20 CRKG1020 101: C C 102: C IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING CF ACCURACY CRKG1020 104: 16 DO 17 I=1,NDIM CRKG1020 105: 17 AUX(4,I)=Y(1) CRKG1050 106: ITEST=1 CRKG1050 107: ISTEP=ISTEP+ISTEP=2 CRK01070	93:		IF(J-3) 13, 14, 13	CRKG 930
95: 14 CALL FCT(Y,NDIM,DERY,PW) CRKG 550 56: GOTO 10 CRKG 960 97: C CRKG 973 98: C TEST OF ACCURACY DRKG 933 59: C DRKG 935 10: 15 IF(ITEST)16,16,20 CRKG1020 101: C C 102: C IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING CF ACCURACY CRKG1020 104: 16 DO 17 I=1,NDIM CRKG1030 105: 17 AUX(4,I)=Y(I) CRKG1050 106: ITEST=1 CRKG1050 107: ISTEP=1STEP+1STEP=2 CRKG1020	74:		13 X=X+.5D0*H	ERKG 947
56: GOTO 10 C	95:		14 CALL FCT(Y,NDIM,DERY,PW)	CRKG 550
97: C C CRKG 971 98: C TEST OF ACCURACY DRKG 933 99: C DRKG 992 130: 15 IF(ITEST)16,16,20 CRKG1020 101: C C 102: C IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING CF ACCURACY CRKG1020 103: C C 104: 16 DO 17 I=1,NDIM CRKG1020 105: 17 AUX(4,I)=Y(I) CRKG1050 106: ITEST=1 CRKG1050 107: USTEP=ISTEP+ISTEP=2 CRKG1050	96 :		GOTO 10	CRKG 960
98: C TEST OF ACCURACY DRKG 930 59: C DRKG 990 100: 15 IF(ITEST)16,16,20 DRKG1020 101: C DRKG1020 102: C IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING CF ACCURACY DRKG1020 103: C DRKG1020 DRKG1020 104: 16 D0 17 I=1,NDIM DRKG1020 DRKG1040 105: 17 AUX(4,I)=Y(I) DRKG1050 DRKG1050 106: ITEST=1 DRKG1050 DRKG1050 107: ISTEP=ISTEP+ISTEP=2 DRKC1070	97:	С		CRKG 970
\$9: C DRKG \$9C 1J0: 15 IF(ITEST)16,16,20 DRKG1C0 L01: C DRKG1C10 L02: C IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING CF ACCURACY DRKG1020 L03: C DRKG1020 L04: 16 D0 17 I=1,NDIM DRKG1020 L05: 17 AUX(4,I)=Y(I) DRKG1050 L06: ITEST=1 DRKG1050 L07: ISTEP=ISTEP+ISTEP=2 DRKC1070	98:	Č	TEST OF ACCURACY	DRKG 931
130: 15 IF(ITEST)16,16,20 ERKG1000 L01: C ERKG1010 L02: C IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING CF ACCURACY DRKG1020 L03: C ERKG1030 L04: 16 D0 17 I=1,NDIM ERKG1040 L05: 17 AUX(4,I)=Y(I) ERKG1050 L06: ITEST=1 ERKG1060 L07: ESTEP=ISTEP+ISTEP=2 ERKG1070	99:	č		CRKG 990
LUI: C LUI: C	100:	•	15 IE(ITEST)16.16.20	LEKG1000
LC2: C IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING CF ACCURACY DRKG1020 L03: C DRKG1020 DRKG1020 L04: 16 D0 17 I=1,NDIM DRKG1040 DRKG1050 L05: 17 AUX(4,I)=Y(I) DRKG1050 DRKG1050 L06: ITEST=1 DRKG1060 DRKG1060 L07: USTER=ISTER+ISTER=2 DRKG1070	101:	C		ERKG1010
Li2 G Li2 G Li2 DRKG1/2G Li3: C C DRKG1/3C DRKG1/3C L04: 16 D0 17 I=1,NDIM DRKG1/5C L05: 17 AUX(4,I)=Y(I) DRKG1/5C DRKG1/5C L06: IT_CST=1 DRKG1/5C DRKG1/5C L07: LSTEP=ISTEP+ISTEP=2 DRKG1/5C	102:	č	IN CASE ITESTED THERE IS NO POSSIBILITY FOR TESTING OF ACCURACY	
L04: 16 D0 17 I=1,NDIM DRKC1040 L05: 17 AUX(4,I)=Y(I) DRKG1050 L06: ITcST=1 DRKG1060 L07: LSTEP=ISTEP+ISTEP=2 DRKC1070	1.3:	č	IN ORGE ITEST & THERE IS NO FOSSIBLEIT FOR TESTING OF FOODRAGT	CRKC1C32
105: 17 AUX(4,I)=Y(I) 106: ITEST=1 107: ISTEP=ISTEP+ISTEP-2	104:	Ŭ	16 PO 17 I=1.NDIM	
LG: ITcST=1 LG: ISTEP=ISTEP+ISTEP=2 LG: ISTEP=ISTEP+ISTEP=2	1.25:		$17 \text{ AUX}(4 \cdot 1) = Y(1)$	DRKG1(ST
	166:			
	167:		ISTEP=ISTEP+ISTEP-2	ERKC1C70

108.		18 1416-1416-1	50KC1C90
100:			
11.1.1			
111.			
111.			URKGIIIO
112:		Y(1) = AUX(1,1)	ERKG1120
113:		LERY(1) = ALX(2, I)	DRKG113J
114:		15 AUX(6,I) = AUX(3,I)	DRKG114C
115:		GUTO 9	ERKG1150
116:	С		ERKG116J
117:	С	IN CASE ITEST=1 TESTING OF ACCURACY IS POSSIBLE	DRKG117U
118:	С		CRKG118C
119:		20 IMOD=ISTEP/2	CRKG1190
120:		IF(ISTEP-IMOD-IMOD)21,23,21	DRKG12CC
121:		21 CALL FCT(Y,NDIM,DERY,PW)	DRKG121C
122:		CO 22 I=1.NDIM	
123:		AUX(5,T)=Y(T)	DEKG1231
124:		22 AUX(7.1)= $CERY(1)$	DRKG124C
125:		GOTO S	
126:	C		
127:	č	COMPLITATION OF TEST VALUE DELT	
128:	ñ	CERTORATION EL TEST VALOE DELL	
120:	C	23 DELT-0 DO	
130.			
121.		$\frac{1}{2}$	
122+		$\frac{24}{16} \frac{1}{16} $	DRKGISIC
102.	c	1F(UELI-PRF1(4))20,20,20	LRKG1325
1324	ι c		URKG133J
134:	L C	ERPER IS TOO GREAT	CRKG134C
135:	C		CRKG1350
136:		25 IF(IHLF-1C)26,36,36	CRK G1360
137:		26 DO 27 I=1,NCIM	DRKG137C
138:		27 AUX(4,I) = AUX(5,I)	CRKG138C
139:		ISTEP=ISTEP+ISTEP-4	CRKG1390
147:		X = X - H	DRKG14CC
141:		IEND=C	DRKG1410
142:		GUTO 18	CRKG142C
143:	С		DRKG1430

			PAGE 5
144:	С	RESULT VALUES ARE GOUD	CRKC1440
145:	С		CRKG145C
146:		28 CALL FCT(Y,NCIM,DERY,FW)	DRKG146C
147:		DO 29 I=1,NDIM	CRKG1470
148:		$\Delta \cup X (1, I) = Y (I)$	DRKG1480
149:		AUX(2,I) = EERY(I)	DRKG149C
150:		AUX(3,I) = AUX(6,I)	CRKG1500
151:		$Y(I) = \Delta U X(5, I)$	ERKG1510
152:		29 DERY(I) = AUX(7, I)	DRKG1520
153:		IF(PRMT(5))4C,3C,4C	CRKG1530
154:		30 CO 31 I=1,NDIM	ERKG1540
155:		Y(I) = AUX(1, I)	DRKG1550
156:		31 DERY(I)=ALX(2,I)	DRKG1560
157:		IREC=IHLF	ERKG1570
158:		IF(IEND)32,32,39	DRKG1580
159:	С		DRKG1590
160:	С	INCREMENT GETS DOUBLED	CRKG1679
161:	С		CRKG1610
162:		32 IHLF=IHLF-1	DRKG1620
163:		ISTEP=ISTEP/2	DRKG1630
164:		F=H+H	ERKG1640
165:		IF(IHLF)4,33,33	DRKG165C
166:		33 IMOD=ISTEP/2	DRKG1660
167:		IF(ISTEP-IMOD-IMOD)4,34,4	DRKG1670
168:		34 IF(DFLT 12C1*PRMT(4))35,35,4	DRKG1680
169:		35 IHLF=IHLF-1	DRKG169C
170:		I STEP=I STEP/2	ERKG1700
171:		H = H + F	CRKG1710
172:		GOTO 4	DRKG172C
173:	С		DRKG1730
174:	С	RETURNS TO CALLING PRUGRAM	ERKG1740
175:	С		DRKG1753
176:		36 IHLF=11	CRKG176C
177:		CALL FCT(Y,NDIM,DERY,PW)	CRKG1770
173:		GCTO 39	DRKG178C
179:		37 IHLF=12	DRKG1790

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180:		GOTC 39	DRKG18CC
181:	38	IHLF=13	DRKG1810
182:	39	CONTINUE	CRKG1820
183:		PRMT(1) = X	DRKG1830
184:	51	FORMAT(2(/),20X,*X =*,F16.12,10X,*IHLF =*,I5)	DRKG1840
185:	40	RETURN	CRKG1850
186:		ENC	CRKG186)

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PAGE

1:			SUBRCUTINE FCT(YP,M,DY,PW)	FCT	10
2:	С			FCT	20
3:	C			FCT	30
4:	С		THIS SUPRLUTINE COMPUTES THE DERIVATIVES (RIGHT HAND SIDES)	FCT	4)
5:	С		OF THE SYSTEM TO GIVEN VALUES OF YP(CONCENTRATION)	FCT	50
6:	С			FCT	60
7:	С			FCT	70
8:			IMPLICIT REAL*8(A-H,O-Z)	FCT	6.0
9:			DIMENSION YP(M), DY(M), PW(M, M)	FCT	90
10:			DU 15 J=1,M	FCT	100
11:			$DJO \cdot D = O$	FCT	110
12:			DO 1º I=1,M	FCT	120
13:		10	DY(J) = DY(J) + PW(J,I) + YP(I)	FCT	130
14:		15	CONTINUE	FCT	140
15:			RETURN	FCT	150
16:			-ND	FCT	160

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1:		SUBROUTINE VELDIF(XZ,H,UGR,UST,AM,U,V,ISTE,ALPHA,N3,AKY,AKZ,EAKZ,	VELD	10
2:		1STL, IND, US, DKN, DUN, HSKN, HGEO, AMM)	VELC	27
3:	С		VELD	30
4:	С		VELD	46
5:	С	THIS SUBROUTINE CALCULATES THE VELOCITY AND TURBULENT	VELC	50
6:	С	CIFFUSIVITY VECTORS (TWO-DIMENSIONS) AS FUNCTIONS OF	VELD	60
7:	С	ELEVATION AND STABILITY CLASS	VELD	70
8:	С		VELC	80
9:	С		VELD	90
17:		IMPLICIT REAL*8(A-H,O-Z)	VELD	100
11:		DIMENSION XZ(12),AKY(12),AKZ(12),DAKZ(12),CCEFK(6),DKN(6),	VELC	110
12:		1TDFKN(6),CUN(6),TDFUN(6),U(12),V(12),HGEC(6)	VELC	120
13:		DATA COEFK/570.D0,555.D0,540.D0,222.D),0.DC,-7J.5D0/	VELD	133
14:		IF(IND.NE.C) GC TC 5	VELC	140
15:		US=UST*(1.DO-DFXP(-SFL*H/AM)*DCOS(SEL*H/AM))	VELD	150
16:		PETURN	VELD	160
17:		5 CONTINUE	VELD	173
18:		TDFKN(ISTB)=DKN(ISTB)/H	VELC	187
19:		U(1)=UGR	VELD	190
26:		PV=DEXP(-CKN(ISTB)/AM)*DSIN(DKN(ISTE)/AM)/	VELD	200
21:		1(1.DC-DEXP(-DKN(ISTB)/AM)*DCCS(DKN(ISTB)/AM))	VELD	210
22:		U1=UST*(1.CC-CCXP(-DKN(ISTB)/AM)*DCOS(DKN(ISTB)/AM))/	VELC	223
23:		1(DKN(ISTP)/DUN(ISTE))**AMM	VELD	230
24:		V(1)=-PV*L(1)	VELD	240
25:		TDFUN(ISTB)=HGEO(ISTB)/H	VELC	250
26:		DO 25 L=2,N3	VELD	26C
27:		l(l)=lST*(1.DG-DEXP(-XZ(L)*H/∆M)*CCCS(XZ(L)*H/AM))	VELD	27C
28:		IF(XZ(L).LE.TDFKN(ISTB)) U(L)=U1*(XZ(L)*F/CUN(ISTB))**AMM	VELD	280
29:		IF(XZ(L).LT.TCFUN(ISTB)) V(L)=-UST*DEXP(-XZ(L)*H/AM)*	VELD	290
3):		1DSIN(XZ(L)*H/AM)	VELD	300
31:		$IF(XZ(L) \cdot GE \cdot TDFUN(ISTB)) V(L) = C \cdot D^{\circ}$	VELD	311
32:		IF(XZ(L).LT.TCFKN(ISTB)) V(L)=-PV*U(L)	VELD	ר 32
33:		25 CONTINUE	VELD	33U
34:		IF(ISTB.GE.5) GO TO 10	VELC	34)
35:		IF(DKN(ISTR).GT.1.D-CR) GU TO 20	VELC	357

36:		DO 4 L=2,N3	VELD 360
37:		AKZ(L)=CUEFK(ISTB)+90.DO	VELD 370
38:		$DAKZ(L) = U \cdot CO$	VELD 380
39:	4	AKY(L)=ALPHA*AKZ(L)	VELD 390
40:		RETURN	VELC 402
41:	2 1	CONTINUE	VELD 41.
42:		TDSKN=1.DC-1CC.DC/H	VELD 420
43:		IF(H.LE.HSKN) TDSKN=1.DO	VELD 430
44:		CC 2 L=2,N3	VELD 446
45:		IF(XZ(L)-TDFKN(ISTP)) 11,12,12	VELD 450
46:	11	AKZ(L)=COEFK(ISTB)*XZ(L)/TDFKN(ISTB)+90.DC	VELD 460
47:		EAKZ(L)=CCEFK(ISTB)/CKN(ISTB)	VELD 470
48:		GO TC 16	VELD 48C
49:	12	IF(XZ(L)-TDSKN) 13,13,14	VELD 490
51:	13	AKZ(L)=CUEFK(ISTB)+9C.DC	VELC 500
51:		$DAKZ(L) = 2 \cdot DQ$	VELD 510
52:		GO TO 15	VELD 527
53:	14	AKZ(L)=COEFK(ISTR)*H*(1.DC-XZ(L))/1CC.DC+SC.DO	VELD 530
54:		DAKZ(L)=-CCEFK(ISTB)/100.CO	VELD 543
55:	15	CONTINUE	VELD 556
56:	16	AKY(L)=ALPHA*(COEFK(ISTB)+9C.DC)	VELD 560
57:	2	CONTINUE	VELD 570
58:		GD TO 50	VELD 580
59:	10	CONTINUE	VELC 591
60:		$EO_{3} L=2, N3$	VELD 600
61:		AKZ(L)=CCEFK(ISTB)+90.C)	VELD 610
62:		$DAKZ(L) = 3 \cdot DC$	VELD 620
63:	٦	AKY(L)=ALP⊢A*AKZ(L)	VELC 630
64:	5 1	CONTINUE	VELD 643
65:		RETURN	VELD 650
66:		END	VELD 660

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С
С
С
      INPUT DATA RECUIRED
C
C
  10 10 4
    4220400+00
                                                   8.90000+00
                                                                     0.0
                     500.00+00
                                   4000.00+00
     687.22D+C'
                    322.490+00
                                     30.00+00
                                                   60.0000+00
                                                                    0.20
 FC.CP+00 50.CD+C0 50.0D+C0
                                50.0D+00 50.0D+00 50.0D+00
 1 /. ^ C + 00 10.6 C + 00 10.9 C + 30
                                10.UC+00 10.0C+CC 10.CD+CC
147.350+ 1145.670+01143.970+01101.310+01544.140+00253.280+00
                                      2.1D-06
                       6.1D-C6
                                                    1.0000-07
         •CD+CC
      .29610-02
                     ·2861D-02
                                      0.1D-01
                                                    0.0120-01
      ·29610-J2
                     •2061 C-72
                                     0.120-02
       C.CD+CL
                                     C.25D-02
                                                    0.250-62
                      (.1D-C6
      ·25000-02
                     .2500D-02
                                  1500.0D+00
                                                     C. 14D+CC
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APPENDIX B

NOMENCLATURE

a	Constant in equation (3.14)
A _{ij}	Element of the discretizational matrix of first derivatives
B _{ij}	Element of the discretizational matrix of second derivatives
С	Mean concentration, mg/m^3
C _a	Mean concentration obtained by an analytical solution
C _c	Mean concentration calculated by the present work
C _i	Mean concentration at the i-th interior orthogonal collocation point - two-dimensional models
C _o	Equivalent mean concentration at the source
C _{kl}	Mean concentration at the interior orthogonal collocation point (n_k, ζ_l) - three-dimensional models
e	Absolute error defined by equation (3.1), %
E _{ij}	Elements of the collocation matrix
f	Coriolis parameter, sec ⁻¹
Н	Effective emission height, m
^k 1	Reaction rate constant, min ⁻¹
К	Turbulent diffusivity, m ² /sec
К ₁	Turbulent diffusivity at an elevation z ₁
m	Exponent in power-law form for the mean wind velocity profile
n	Exponent in power-law form for the turbulent diffusivity profile
N	Number of interior orthogonal collocation points.

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р	Atmospheric pressure
Q	Source strength, kg/sec unless otherwise specified
$Q_{\mathbf{x}}$	Mass rate through y-z plane at x=constant, gm/sec unless otherwise specified
r	Parameter in equation (2.9)
r	Mathematical parameter that represents the ratio of boundary to centerline concentration
R	Rate of generation of species
S	Parameter in equation (2.9)
t	Time, sec
u	Mean wind velocity in the x-direction, m/sec unless otherwise specified
^u 1	Mean wind velocity at an elevation z_1
^u 10	Mean wind velocity at 10 meters
Ū	Eigenvectors of matrix E
<u></u>	Eigenrows of matrix E
ν	Mean wind velocity in the y-direction, m/sec unless otherwise specified
W	Mean wind velocity in the z-direction, m/sec unless otherwise specified
W	Quadrature weights
x	Cartesian coordinate in mean wind direction, m unless otherwise specified
x _{max}	Maximum distance in the x-direction, m
у	Cartesian coordinate in lateral direction, m
y _{max}	Maximum distance in the y-direction, m

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Z	Cartesian coordinate in vertical direction, m
^z max	Maximum height above terrain (in some cases refers to the elevation of the inversion layer), m
^z 1	Reference height, m

Greek Symbols

α	Angle between geostrophic velocity and surface boundary layer velocity, $^\circ$
β	Mathematical parameter that represents a source dimension
Г	Gamma function
δ	Mathematical parameter used for spatial variable transformations
δ _{ij}	Kronecker delta function
Δ	Knee height for the vertical turbulent diffusivity profile, m
ε	Upper error bound in "DRKGS"
ζ	Dimensionless spatial variable in the z-direction
η	Dimensionless spatial variable in the y-direction
₫	Eigenvalues of matrix E
ξ	Dimensionless spatial variable in the x-direction
ρ	Density
σ	Standard deviation
τ	Eddy stresses
φ	Geostrophical latitude, °
ψ	Variable used in Figure 4.6. Represents ground-level concen- tration

Superscripts

i	Initial	value	profile	for	the	concentration
*	Refers t	o dime	ensionles	s sp	atia	l variables

Subscripts

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