AN ANALYSIS OF FINITE DIFFERENCE AND GALERKIN TECHNIQUES APPLIED TO THE SIMULATION OF ADVECTION AND DIFFUSION OF AIR POLLUTANTS FROM A LINE SOURCE

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PREFACE

Management of environmental quality very often has to deal with the analysis of transport and diffusion of pollutants. In most cases, the process is nonstationary and its simulation requires the numerical solution of the time dependent continuity equation.

The fundamental problem of the error introduced by the discretization on a computer of time dependent processes of transport and diffusion of pollutants is addressed in this study with specific reference to dispersion of air pollutants from an elevated source.

This work is part of the activity of the Resources and Environment Area (Task 2 Environmental Quality Control and Management) on application and evaluation of air pollution models. It was conducted jointly with the IBM Italy Scientific Center of Rome and the Max Planck Institut für Plasmaphysik of Garching bei München.

ABSTRACT

A finite difference and a Galerkin type scheme are compared with reference to a very accurate solution describing time dependent advection and diffusion of air pollutants from a line source in an atmosphere vertically stratified and limited by an inversion layer.

The accurate solution was achieved by applying the finite difference scheme on a very refined grid with a very small time step. Grid size and time step were defined according to stability and accuracy criteria discussed in the text.

It is found that for the problem considered, the two methods can be considered equally accurate. However, the Galerkin method gives larger areas of small errors close to the source. This was assumed to be partly due to the different way the source term is taken into account by the two methods. An improvement of the accuracy of the finite difference scheme was achieved by approximating, at every step, the contribution of the source term by a Gaussian puff moving and diffusing with velocity and diffusivity of the source location, instead of utilizing a stepwise function for the numerical approximation of the δ function representing the source term.

CONTENTS

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INTRODUCTION

Simulation of advection and diffusion of pollutants in environmental media are required for the definition of both planning and control strategies. In many situations, the problem is the dispersion of pollutants from a point source in a turbulent flow. A classical mathematical model of this process is provided by the continuity equation which, neglecting removal processes, takes the form:

$$\frac{\partial C}{\partial t} + \underline{\nabla}\cdot(\underline{U}\,C) = \underline{\nabla}\cdot(\overline{\overline{K}}\cdot\underline{\nabla}C) + Q\delta(\underline{x} - \underline{x}_s) \qquad (1)$$

In (1), C is the mean (ensemble average) concentration of the considered pollutant, $\underline{U}$ is the mean flow velocity vector, $\overline{\overline{K}}$ is the turbulent diffusivity tensor, Q is the emission rate of the point source located at (x_s, y_s, z_s) and $\delta(\bullet)$ is Dirac's function.

Equation (1) is based on the mixing length or gradient transport hypothesis (see Leslie, 1973) which, by analogy with molecular diffusion, assumes that the turbulent flux can be expressed as the

product of an eddy diffusivity coefficient and the gradient of the mean concentration. The gradient transfer hypothesis implies that equation (1) can only resolve spatial and temporal variations of the concentration on scales larger than the respective Lagrangian scales of the turbulence.

Limitations of the gradient transfer hypotheses are discussed by Corrsin (1974), Lamb and Seinfeld (1973), and other researchers. The present study is concerned with the problem of solving (1) by numerical methods. Both a finite difference and a Galerkin scheme have been used to simulate numerically the processes described by (1). The schemes considered are compared with reference to their application to the classical two-dimensional problem of dispersion of air pollutants from an elevated line source in the atmospheric boundary layer. For this specific problem, the finite difference scheme is used to compute a very accurate solution by solving (1) on a highly refined grid and using an extremely small integration time step. The finite difference and the Galerkin schemes are then applied to solve the same problem on much coarser grids with larger time steps; then the results are compared with the refined solution. Finally, an improved method of treating the source term of (1), when finite difference schemes are applied, is discussed.

REFERENCE CASE

The numerical schemes in this study have been applied to a problem which can be considered a mathematical description of the dispersion of an inert air pollutant from a crosswind line source of infinite extent and uniform emission in an atmosphere vertically limited by an inversion layer. For this problem,

if the x-axis is taken along the wind vector (assumed to have components only in the horizontal plane), the y-dependent terms of (1) can be eliminated. Assuming also that the axes of the chosen frame of reference are the principal axes of the diffusivity tensor and that ground and inversion layers completely reflect the diffusing material, the mathematical formulation of the problem can be stated as:

$$\frac{\partial C}{\partial t} + U(z)\frac{\partial C}{\partial x} = K_x \frac{\partial^2 C}{\partial x^2} + \frac{\partial}{\partial z}\left(K_z \frac{\partial C}{\partial z}\right) + Q\,\delta(z-z_s)\,\delta(x-x_s) \qquad (2)$$

$$K_z \frac{\partial C}{\partial z} = 0 \qquad z = 0,\ H \qquad (2a)$$

$$C(x,z,t) = 0 \qquad x = \pm\infty \qquad (2b)$$

$$C(x,z,t) = 0 \qquad t = 0 \qquad (2c)$$

where H is the height of the inversion layer. Equation (2) is derived from (1) with the additional assumptions of constant horizontal diffusivity and wind and vertical diffusivity as functions only of the vertical coordinate. In formulating the boundary value problem (2)-(2c), the region is considered unpolluted at time t = 0.

To generalize results given by the numerical solution to equation (2) and related boundary and initial conditions (2a)-(2c), the variables and parameters x, z, t, U, K_x, K_z, C have been expressed respectively in units of $\frac{H^2 U(H)}{K_2(H)}$, H, $\frac{H^2}{K_2(H)}$, U(H), $\frac{H^2 U^2(H)}{K_2(H)}$, $K_2(H)$, $\frac{Q}{U(H)\cdot H}$. Use of these normalizing factors leaves equations (2)-(2c) formally unchanged except for the emission rate and the inversion layer height, which are both normalized to unity.

An accurate solution to the problem described by (2)-(2c) (with given wind and diffusivity) has been computed by means of the finite difference scheme described below.

Finite Difference Scheme

The finite difference scheme used is based on the method of fractional steps (see, e.g., Yanenko, 1971). According to this procedure, (2) is split into the following sequence of one-dimensional equations:

$$\frac{\partial C}{\partial t} = \delta(x-x_s)\delta(z-z_s) \tag{3a}$$

$$\frac{\partial C}{\partial t} = -U \frac{\partial C}{\partial x} \tag{3b}$$

$$\frac{\partial C}{\partial t} = K_x \frac{\partial^2 C}{\partial x^2} \tag{3c}$$

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}\left(K_z \frac{\partial C}{\partial z}\right) \tag{3d}$$

At each time step, the above equations are solved sequentially by taking as initial concentration the one obtained by solving the previous equation. Each of the above equations is numerically integrated over the time step Δt. The concentration field obtained after the integration of (3d) is the numerical solution to the boundary value problem (2)-(2c) after the considered time step and provides the initial condition to (3a) for the next time step. In practice, the processes described by (3a)-(3d) are considered separate occurrences at each time step. Reduction of the integration time step decreases the error introduced by this assumption.

The fractional step procedure has been extensively applied to a problem similar to that discussed here (Shir and Shieh (1974), Runca and Sardei (1975), and Runca et al. (1979)). A geometric interpretation of the procedure described above follows.

The trajectory of the pollutant particle (Fig. 1) starts from a at time $n\Delta t$ and reaches the grid point b(i,k) at time $(n + 1)\Delta t$. Its concentration at point b can be expressed as:

$$C_b = C_a + \Theta \tag{4}$$

where Θ is the contribution due to diffusion processes. (From here on it is assumed to operate over points of the integration grid which do not include the source term.)

By defining C^* as the value of the concentration field that would be found at time $(t + \Delta t)$ if no diffusion occurs, C^{**} as the field obtained if no vertical diffusion occurs, and A, D_x, and D_z as the finite difference explicit operators for advection, horizontal, and vertical diffusion respectively, (3b)-(3d) yield at point b(i, k):

$$C_b^* = A[C_{ik}^n] \simeq C_a \tag{5a}$$

$$C_b^{**} = C_b^* + D_x[C_b^*] \tag{5b}$$

$$C_b \simeq C_{ik}^{n+1} = C_b^{**} + D_z[C_b^{**}] \tag{5c}$$

Equations (5a)-(5c) show that by virtue of the fractional step procedure, the contribution Θ given by the diffusion processes is evaluated with respect to point a, which belongs to the trajectory of the pollutant particle. As pointed out by Sardei and Runca (1975), this would not have occurred if (2) had not been

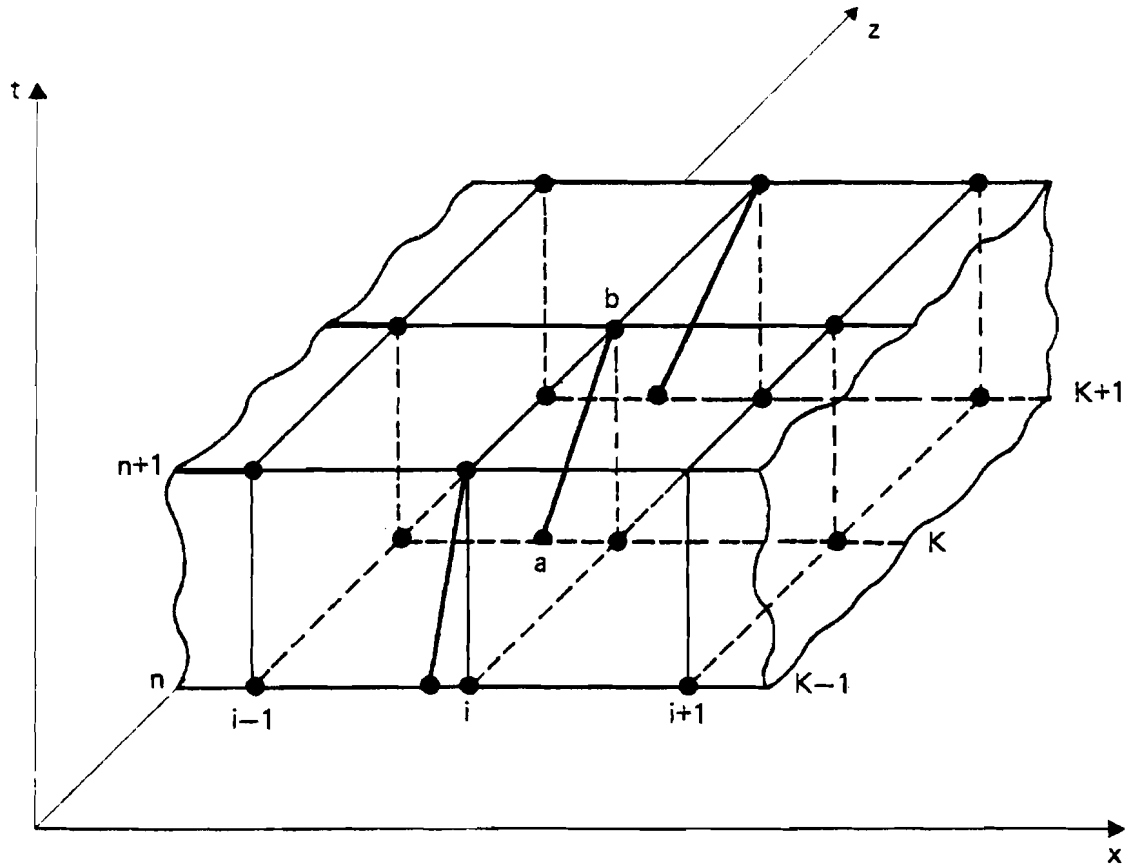

Figure 1. Geometric description of the finite difference scheme. ab is the trajectory of the pollutant particle at level z_k.

divided into (3a)-(3d). This property of the fractional step procedure (that of evaluating the diffusion contribution Θ on points belonging to the trajectory of the pollutant particle, thus retaining the Lagrangian aspect of the processes described by (1)) is better expressed if the Crank-Nicolson scheme is adopted for the approximation of the diffusion terms. In this case, (5a)-(5c) can be combined to produce the equation:

$$C_b \simeq C_{ik}^{n+1} = C_a^* + \frac{1}{2}\left\{D_x[C_b^{**}] + D_x[C_a^*]\right\} + \frac{1}{2}\left\{D_z[C_b] + D_z[C_a^*]\right\}$$

$$+ \frac{1}{4}\left\{D_z D_x[C_b^{**}] + D_z D_x[C_a^*]\right\} \quad . \tag{6}$$

$C_a^* \equiv C_b^* \equiv A[C_{ik}^n]$ has been used to point out better at which location of the pollutant trajectory the numerical scheme operates. Note that the terms $D_x D_z[\bullet]$ can be interpreted as representative of the interaction between the horizontal and the vertical diffusions.

Equation (6) is implemented in this study. In order to program the scheme elucidated above, the operators U, D_x, and D_z must be defined.

Much attention was paid to the development of a numerical scheme which can avoid the amplitude and phase errors from the approximation of the advective terms of (1) (equation (3b) in the case considered here). A summary of the proposed methods can be found in Berkowicz and Prahm (1979). In the present study, the choice is made to approximate equation (3b) by the Lax-Wendroff scheme (Richtmyer and Morton (1967)). By choosing the Lax-Wendroff scheme, $C_a^* \equiv C_b^*$ is the value obtained in "a" through parabolic interpolation over the points (i - 1, k), (i, k), and (i + 1, k).

The adopted diffusion operators were the usual second-order centered difference operators.

Under the stated conditions, the fractional step procedure described by (3a)-(3d) is used to solve the boundary value problem (2)-(2c). However, in order to do that, appropriate boundary conditions must be chosen for the single steps (3b)-(3d) and step (3a) must be numerically approximated.

In the problem dealt with, the boundary conditions for (3b)-(3d) are easily determined. For (3d), the boundary conditions are given by (2a), while for (3b)-(3c), the extent of the integration grid is assumed to be such that the concentration can be considered equal to zero both at the downwind and at the upwind lateral boundaries.

The numerical approximation of (3a) is obtained, as usual, by adding a contribution at each time step to the points close to the source location so that the total matter in the region increases by $Q\ \Delta t$ (Δt in normalized units). This method introduces large errors close to the source. An improved way of treating the source term is therefore shown later.

The scheme described above is used in order to compute an accurate solution to the boundary value problem (2)-(2c) for realistic wind and diffusivity profiles (explained in the section "Refined Solution").

Accuracy Conditions

Here, accuracy conditions to be met in applying the discussed finite difference scheme are reviewed. The application of Von Neuman's stability analysis to the above fractional step procedure shows that the amplification factor of a Fourier concentration

component is the product of the amplification factors of the single steps (Roache (1972)). The stability condition required by the scheme is, therefore, only the Courant condition.

$$\frac{u\Delta t}{\Delta x} < 1 \tag{7}$$

This stems from the use of Lax-Wendroff's scheme for the advection step.

No conditions are introduced by the diffusion steps since Crank-Nicolson's scheme is unconditionally stable. However, in order to avoid negative amplification factors of the high-order Fourier components in the derivation of the accurate numerical solution, the following conditions are also required:

$$\frac{K_x \Delta t}{\Delta x^2} \leq \frac{1}{2} \tag{8}$$

$$\frac{K_z \Delta t}{\Delta z^2} \leq \frac{1}{2} \quad . \tag{9}$$

Another condition is also imposed on the grid geometry and time steps to guarantee the derivation of an accurate numerical solution. In order to illustrate this condition, let us consider the one-dimensional equation:

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = K_x \frac{\partial^2 C}{\partial x^2} \quad .$$

Application of the Lax-Wendroff and Crank-Nicolson schemes to this equation give:

$$C_i^{n+1} - C_i^n = -\frac{\alpha}{2}(C_{i+1}^n - C_{i-1}^n) + \frac{\alpha^2}{2}(C_{i+1}^n - 2C_i^n + C_{i-1}^n) + \frac{1}{2}\beta[(C_{i+1}^n - 2C_i^n + C_{i-1}^n) + (C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1})]$$

where

$$\alpha = \frac{u\Delta t}{\Delta x}$$

and

$$\beta = \frac{K_x \Delta t}{\Delta x^2} \quad .$$

The above equation can be rearranged as follows:

$$C_i^{n+1} - C_i^n = -\alpha(C_i^n - C_{i-1}^n) + \left(\frac{\beta}{2} - \frac{\alpha}{2} + \frac{\alpha^2}{2}\right)(C_{i+1}^n - 2C_i^n + C_{i-1}^n) + \frac{\beta}{2}(C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1}) \quad ,$$

that is, as a linear combination of an upwind difference scheme and a Crank-Nicolson type of scheme in which the coefficient of the second order centered difference at time $n\Delta t$ is altered by the factor $-\frac{\alpha}{2} + \frac{\alpha^2}{2}$. On purely physical grounds, it seems reasonable

to impose:

$$\beta > \alpha - \alpha^2 \qquad (10)$$

in order to avoid simulation of dispersion processes having negative diffusion coefficients. Condition (10), derived by reducing Lax-Wendroff's scheme to the classical upwind difference scheme, could also be obtained by von Neumann's analysis. By reducing Lax-Wendroff's scheme to the upwind scheme in (6), the coefficient of the centered difference at time $n\Delta t$ is altered as above, and condition (10) is thereby considered in the definition of the grid geometry and the time integration step adopted for the computation of the accurate solution.

Refined Solution

The boundary value problem (2)-(2c) is solved with the above defined scheme for (in normalized units):

$$K_x = 10^4$$

$$K_z = ze^{-4(z-1)}$$

$$U = z^{0.2}$$

over the region $0 < x < 2.4 \cdot 10^{-2}$ and $0 < z < 1$.

The chosen vertical eddy diffusivity is the same as that adopted by Shir and Shieh (1974); it can be considered representative of diffusion in a neutral atmosphere (Shir (1973), Wyngard et al. (1974), Robins (1978)).

The integration region has been described by 481 points in the horizontal axis and 97 in the vertical axis, corresponding to $\Delta x = 0.00005$ and $\Delta z \cong 0.0104$ respectively. Using $\Delta t = 0.0000125$,

the following values are obtained for conditions (7)-(10).

$$\frac{U_{max}\Delta t}{\Delta x} = 0.25$$

$$\frac{K_x \Delta t}{\Delta x^2} = .5$$

$$\frac{K_{z_{max}} \cdot \Delta t}{\Delta z^2} \cong 0.58$$

$$\frac{K_x \Delta t}{\Delta x^2} > \left[\frac{U\Delta t}{\Delta x}\left(1 - \frac{U\Delta t}{\Delta x}\right)\right]_{max} = 0.1875$$

Of conditions (7)-(10), only the condition on the vertical diffusion is violated in a small region around the maximum of K_z.

With the above parameters and grid geometry, the integration is carried out for 3072 time steps for two different source heights equal to 0.25 and 0.5 respectively. In both cases, the source is located at $x_s = 38 \cdot 10^{-4}$.

As mentioned above, the boundary conditions at both the upwind and downwind lateral extremes of the region assume that the concentration is zero. To avoid the influence of errors introduced by this approximation, the results discussed later refer to the subdomain R of the integration region defined by: $32 \cdot 10^{-4} \leq x \leq 224 \cdot 10^{-4}$.

COMPARISON WITH REFINED SOLUTION

The boundary value problem (2)-(2c) is solved over the same region with the same parameters as specified in the section "Refined Solution", but on coarser grids with larger time steps. The same finite difference scheme delineated above and a Galerkin type of scheme are used. The Galerkin scheme is introduced primarily because of the ease of application when treating complex geometries of the boundaries.

Galerkin Scheme

The Galerkin scheme employed in this study is programmed on the same grid geometry used for the finite difference scheme. A Galerkin scheme similar to the one discussed here has been applied by Melli (1976).

The elements of the rectangular grid representing the region specified in "Rectangular Solution" are divided into triangles by means of diagonals. On the triangular elements thus obtained the set of pyramidal functions ϕ is defined. The concentration is expressed as a linear combination of this set of functions:

$$C^n \simeq \sum_{j=1}^{N} C_j^n \phi_j \qquad (11)$$

where N is the total number of grid points used and C_j is the value of the concentration in the grid points.

By applying the Galerkin principle (Mitchell and Wait (1977)), the following system of ordinary differential equations is obtained:

$$\sum_{j=1}^{N}\left[\iint_{\Omega}\phi_i\phi_j\,dxdz\right]\frac{dC_j}{dt} + \sum_{j=1}^{N}\left[\iint_{\Omega}U\phi_i\,\frac{\partial\phi_j}{\partial x}\,dxdz\right]C_j$$

$$+\sum_{j=1}^{N}\left[\iint_{\Omega}K_x\,\frac{\partial\phi_i}{\partial x}\,\frac{\partial\phi_j}{\partial z}\,dxdz + \iint_{\Omega}K_z\,\frac{\partial\phi_i}{\partial z}\,\frac{\partial\phi_j}{\partial z}\,dxdz\right]C_j$$

$$+\sum_{j=1}^{N}\left[\int_{\Gamma}K_x\phi_i\,\frac{\partial\phi_j}{\partial x}\,\cos\,\hat{x}\underline{n}\,ds\right]C_j = \phi_i(X_s,\,h_s)\quad ;$$

$$i = 1,2,\ldots,N \tag{12}$$

where Ω is the region of integration, Γ is its boundary, s is the curvilinear coordinate along Γ and $\underline{n}$ is the inward unit vector normal to Γ. It must be noted that boundary conditions (2a) have already been used in deriving equation (12), leading to cancellation of integrals along Γ containing vertical diffusion terms. As far as the integrals

$$\int_{\Gamma}K_x\,\phi_i\,\frac{\partial\phi_j}{\partial x}\,\cos\,\hat{x}\underline{n}\,ds$$

are concerned, they are computed in accordance with the assumption that concentration vanishes on lateral boundaries (the same assumption as used for the finite difference scheme).

Discretization of the time derivative by means of the Crank-Nicolson scheme leads to a system of linear algebraic equations which is solved by means of the Seidel iterative technique (Froberg, (1966)). No stability condition is required by this scheme.

Results

In this section, the solutions computed by the Galerkin and the finite difference schemes on coarser grids with larger time steps are compared with the one discussed in the section "Refined Solution". This comparison is carried out in terms of root-mean-square deviations of the solutions given by the two schemes from the refined solution. Specifically, the following normalized value of the root-mean-square of the deviations is used:

$$C_{mean}(t) = \frac{\left\{\frac{1}{A}\iint_R [C(x,z,t) - C_{ref}(x,z,t)]^2 \, dxdz\right\}^{1/2}}{\frac{1}{A}\iint_R C_{ref}(x,z,t) \, dxdz} \qquad (13)$$

where A is the area of the considered subdomain of the integration region. Note that the root-mean-square of the deviations is normalized, at a given time, to the mean concentration of the refined solution, in order to obtain error estimates accounting for the increasing quantity of the total emitted pollutant in the region considered.

The same region over which the refined solution is computed is described successively by 61 x 13 points and 31 x 7 points. Namely, the integration is performed with grid spacing respectively 8 and 16 times larger than the one used in the refined solution. The time steps are made as large as possible without violating the Courant condition, which in the normalized system used, implies $\Delta t \leq \Delta x$. Thus, the time steps are respectively 32 and 64 times larger than the one used for the refined solution.

Considering only the subdomain R as defined in "Refined Solution" (which corresponds to 49 x 13 and 25 x 7 points, respectively), Figure 2 depicts the normalized root-mean-square of the deviations defined by equation (13) for the source located at $z_s = 0.5$.

Figure 2 is constructed by extracting the matrices corresponding to (25 x 7) points from both the refined solution and the one obtained with 61 x 13 points. It shows the behavior with increasing time of the normalized root-mean-square of the deviations computed on (25 x 7) points for both the finite difference (solid lines) and the Galerkin schemes (dashed lines).

The Galerkin scheme results are slightly better than the ones given by the finite difference method. However, if the source height is changed to $z_s = 0.25$, the two schemes give approximately the same result, as shown in Figure 3, which also indicates a reverse situation with respect to Figure 2, i.e., the Galerkin method is not quite as good as the finite difference method.

Both Figures 2 and 3 show that ε_{mean} decreases with time, which indicates a decreasing level of errors in the downwind direction. This is not surprising, since the gradients of the concentration become smaller as the pollutant front moves away from the source. The situation is clearly depicted in Figure 4, which displays the isolines of the percent error

$$\varepsilon_p = |C - C_{ref}| \times 100/C_{ref}$$

for the source located at $z_s = 0.25$ and a grid of 61 x 13 points. In Figure 4, the left side refers to the Galerkin scheme and the right side to the finite difference. Note that in accordance with the above, only the subdomain of (48 x 13) points is utilized.

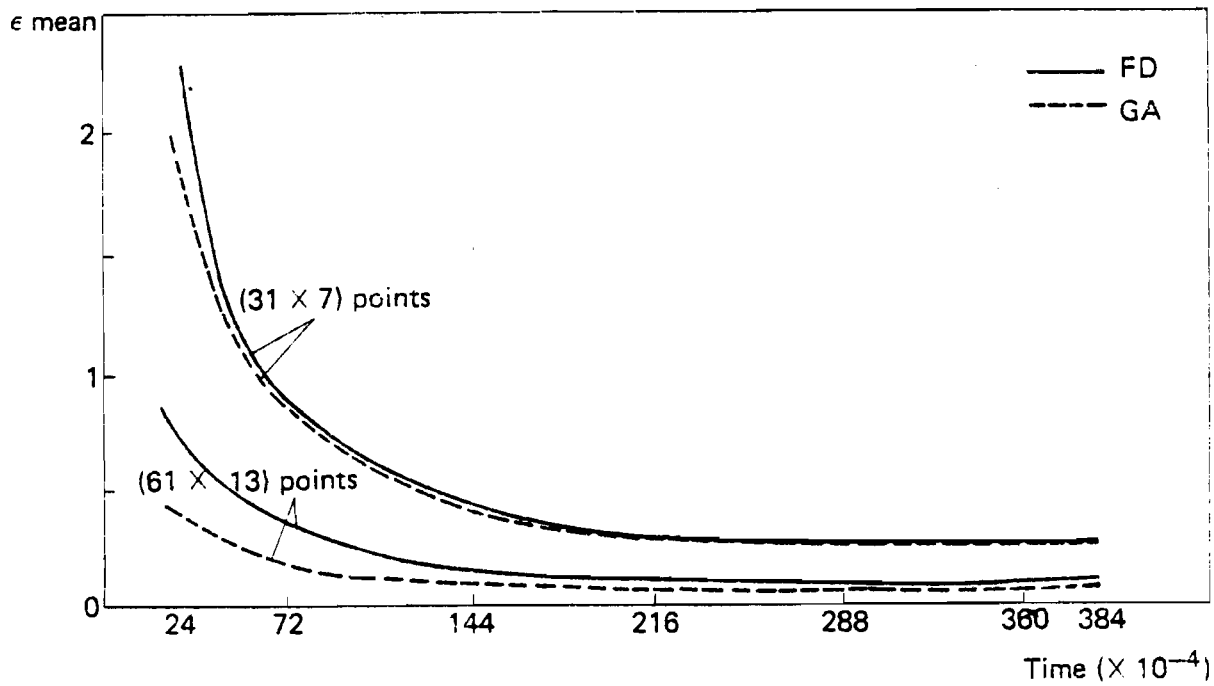

Figure 2. Time evolution of ϵ_{mean} for the finite difference and the Galerkin scheme for grids of (31 x 7) points and (61 x 13) points. In both cases, the time step was taken equal to Δx. Source height = 0.5.

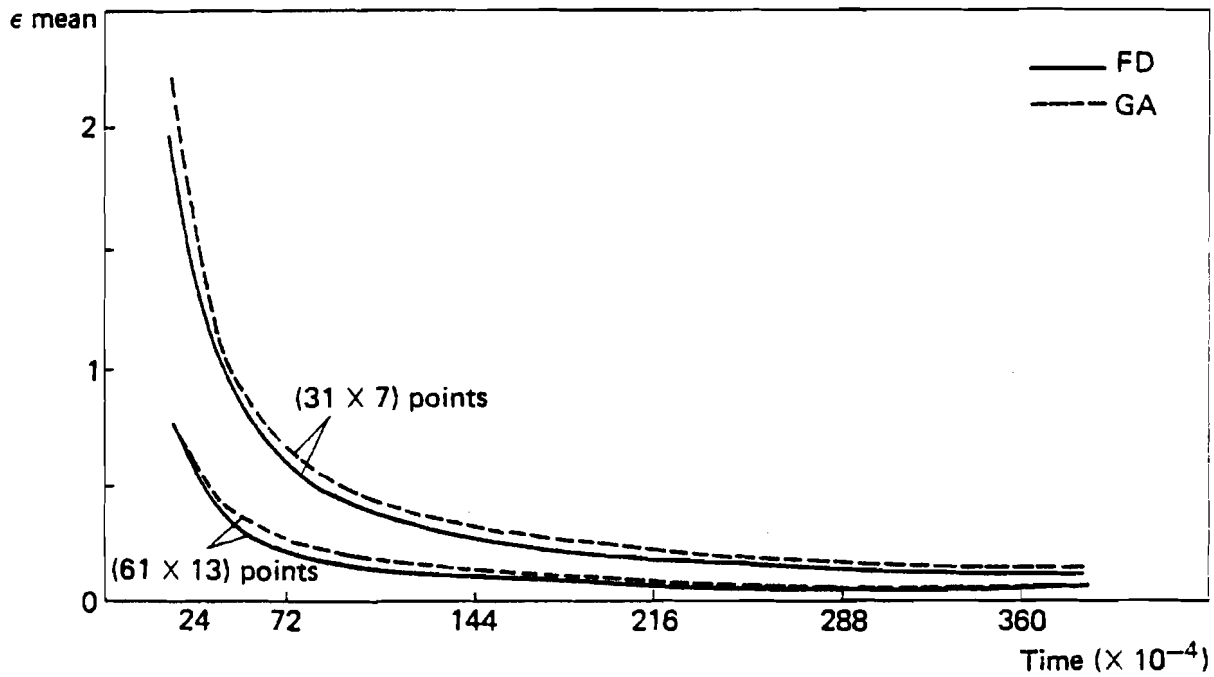

Figure 3. As for Figure 2, except that $z_s = 0.25$.

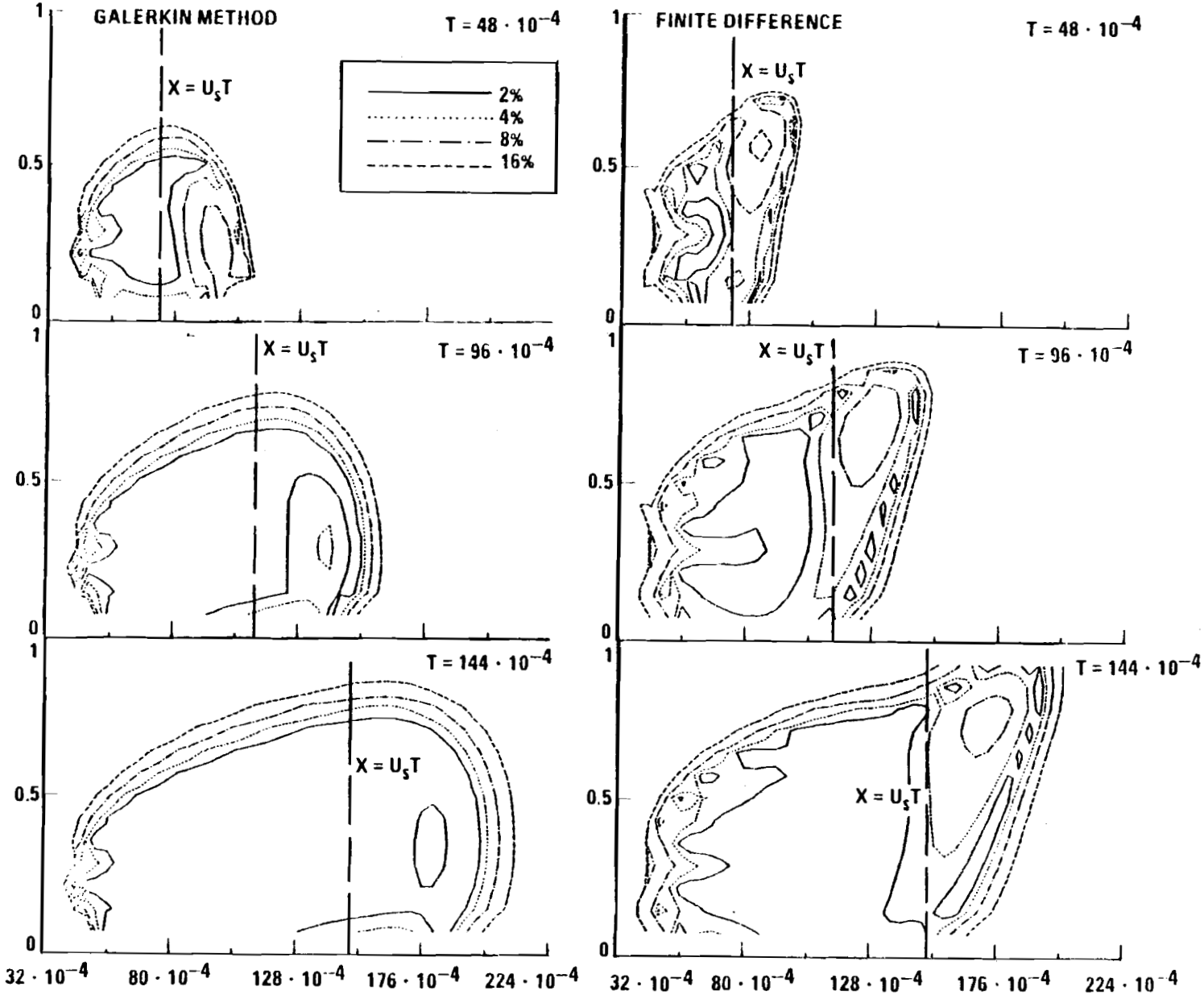

Figure 4. Time sequences of percent error distribution for $z_s = 0.25$. U_s is the wind speed at source height.

The isolines of Figure 4 indicate that the area of small errors increases with increasing simulation time. The Galerkin method shows areas of small errors wider than the ones given by the finite difference scheme. However, it also presents wider areas of larger errors close to the boundaries of the integration region. This explains the results of Figure 3 and the reverse situation with respect to Figure 2. Reducing the source height increases the error induced by the boundaries of the region in the Galerkin method.

The results of Figures 2, 3, and 4 show that a reasonable approximation of the solution of the boundary value problem (2)-(2c) can be achieved with a limited number of points and a large time step for a sufficiently large simulation time. In order to guarantee a sufficiently accurate solution for a small simulation time, especially at points far from the source, the number of grid points must be increased and the time step shortened. It appears from the presented results that in order to avoid errors not much larger than 10% at ground level, the number of grid points should be of the order of (61 x 13) and the time step chosen accordingly. In reality, this is the level of discretization used in applications reported in the literature (Shir and Shieh (1974), Runca et al. (1979)).

On the basis of the above results, the Galerkin method cannot be considered superior to the finite difference scheme. It also requires more computer time since the linear system derived from equation (12) must be solved at every time step. This point is not quantified in this study. By optimizing the solution of the system, the geometry of the grid, and the time step, the computer time required by the Galerkin method can be kept at an acceptable

level. This method can be especially useful in those applications where the boundaries have a complex geometry.

Analysis of Figure 4 also indicates that the Galerkin method approximates, better than the finite difference scheme, the concentration field in the region close to the source, where the maximum gradients of concentration occur. This is because the discontinuity introduced by the source term is somewhat smoothed by the Galerkin method through the integration process leading to equation (12). In the finite difference scheme, the source term is treated "empirically" by adding a contribution to the concentration in the points of the grid close to the source in such a way that at every time step, the quantity Δt is injected in the region. This approach introduces large errors close to the source which, by virtue of the diffusion operator, are smoothed out downwind of the source. Therefore, an improved method of treating the source term to reduce the errors close to the source is discussed next.

Source Term Approximation

Due to the linearity of equation (1), the diffusion process from a point source can be seen at time $n\Delta t$ as the result of two processes. One is the diffusion process of the concentration field C, the other is the diffusion process of the amount of pollutant $\int_{(n-1)\Delta t}^{n\Delta t} Q(t')dt'$ released by the source in the time interval Δt.

The above consideration suggests treating the problem as follows. Let us examine, for the purpose of simplicity, the one-dimensional case:

$$\frac{\partial C}{\partial t} = -U \frac{\partial C}{\partial x} + K_x \frac{\partial^2 C}{\partial x^2} + Q(t)\ \delta(x_s - x) \tag{14}$$

Then, given the equations

$$\frac{\partial C'}{\partial t} = -U \frac{\partial C'}{\partial x} + K_x \frac{\partial^2 C'}{\partial x^2} \quad \text{with } C'^{n-1} = C^{n-1} \tag{15}$$

and

$$\frac{\partial C''}{\partial t} = -U \frac{\partial C''}{\partial x} + K_x \frac{\partial^2 C''}{\partial x^2} \tag{16}$$

with

$$C''^{n-1} = Q^{n-1/2}\ \Delta t\ \delta(x_s - x)$$

it is shown that

$$\left| C'^n + C''^n - C^n \right| = O(\Delta t^2) \tag{17}$$

where C'^n and C''^n are the respective solutions to (15) and (16) at time $n\Delta t$. The sum of $C'^n + C''^n$ by virtue of (17) provides an approximation of C^n.

Not combining (15) and (16) may appear artificial at this point. But separation of these equations allows one to solve (16) by a method different from that used for (15) and furthermore, enables one to experiment with the accuracy of approximation to C^n obtained through integrating (16) only up to a time different by $n\Delta t$. This will be presented later in greater detail.

To prove relation (17), it is convenient to operate in the Fourier space*. If $\tilde{C}$ is the Fourier transform of C in x, relation (17) takes the form:

$$|\tilde{C}'^n + \tilde{C}''^n - \tilde{C}^n| = O(\Delta t^2) \tag{18}$$

Relation (18) can now be proved by considering the following Taylor expansions.

$$\tilde{C}'^n = \tilde{C}'^{n-1} + \Delta t \frac{\partial \tilde{C}'}{\partial t} + \frac{\Delta t^2}{2} \frac{\partial^2 \tilde{C}'}{\partial t^2} + O(\Delta t^3) \tag{19}$$

$$\tilde{C}''^n = \tilde{C}''^{n-1} + \Delta t \frac{\partial \tilde{C}''}{\partial t} + \frac{\Delta t^2}{2} \frac{\partial^2 \tilde{C}''}{\partial t^2} + O(\Delta t^3) \tag{20}$$

$$\tilde{C}^n = \tilde{C}^{n-1} + \Delta t \frac{\partial \tilde{C}}{\partial t} + \frac{\Delta t^2}{2} \frac{\partial^2 \tilde{C}}{\partial t^2} + O(\Delta t^3) \tag{21}$$

By making use of eq. (14-16), the time derivatives of (19)-(21) can be replaced by space derivatives. Recalling that $\frac{\partial \tilde{C}}{\partial x} = ik\tilde{C}$, $\frac{\partial^2 \tilde{C}}{\partial x^2} = -k^2\tilde{C}$ etc., (19)-(21) can be written as follows:

$$\tilde{C}'^n = \tilde{C}'^{n-1} + \Delta t(-iUk - k^2K_x)\tilde{C}'^{n-1} + \frac{\Delta t^2}{2}(-U^2k^2 + 2UK_xk^3 + K_x^2k^4)\tilde{C}'^{n-1} + O(\Delta t^3) \tag{19a}$$

$$\tilde{C}''^n = \tilde{C}''^{n-1} + \Delta t(-iUk - k^2K_x)\tilde{C}''^{n-1} + \frac{\Delta t^2}{2}(-U^2k^2 + 2UK_xk^3 + K_x^2k^4)\tilde{C}''^{n-1} + O(\Delta t^3) \tag{20a}$$

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*In the Fourier space, the transform of Dirac's function and also its derivatives are defined.

$$\tilde{C}^n = \tilde{C}^{n-1} + \Delta t(-iUk - k^2K_x)\tilde{C}^{n-1} + \Delta t\, Q^{n-1}\tilde{\delta}$$

$$+ \frac{\Delta t^2}{2}(-U^2k^2 + 2UK_xk^3 + K_x^2k^4)\tilde{C}^{n-1}$$

$$+ \frac{\Delta t^2}{2}(-iUk - k^2K_x)Q^{n-1}\tilde{\delta} + \frac{\Delta t^2}{2}\left[\frac{\partial Q}{\partial t}\right]^{n-}\tilde{\delta} + O(\Delta t^3) \quad (21a)$$

Recalling that $\tilde{C}'^{n-1} = \tilde{C}^{n-1}$ and $\tilde{C}''^{n-1} = Q^{n-\frac{1}{2}}\Delta t\tilde{\delta}$, the subtraction of equation (21a) from the sum of (19a) and (20a) gives:

$$\tilde{C}'^n + \tilde{C}''^n - \tilde{C}^n = Q^{n-1/2}\Delta t\tilde{\delta} - \Delta t\tilde{\delta}\left(Q^{n-1} + \frac{\Delta t}{2}\left[\frac{\partial Q}{\partial t}\right]^{n-1}\right)$$

$$+ \Delta t^2(-iUk - k^2K_x)Q^{n-1/2}\tilde{\delta}$$

$$- \frac{\Delta t^2}{2}(-iUk - k^2K_x)Q^{n-1}\tilde{\delta} + O(\Delta t^3) \quad (22)$$

Since it is:

$$Q^{n-1} + \frac{\Delta t}{2}\left[\frac{\partial Q}{\partial t}\right]^{n-1} = Q^{n-1/2} - O(\Delta t^2) \quad (23)$$

relation (18) and consequently (17) are proved.

Equations (22) and (23) also indicate that

$$|C'^n + C''^{n-1/2} - C^n| = O(\Delta t^3) \quad (24)$$

However, expansion of the puff in (16) of just $\frac{\Delta t}{2}$ implies that the barycenter of the puff is moved only halfway to its real location. Equation (17) is therefore preferable to equation (24). The numerical tests performed also prove that (17) leads to more accurate results than equation (24).

Equations (15)-(16) and (17) provide an alternative way to treat the source term of equation (1). In fact, assuming that

an approximate solution to equation (16) can be obtained by replacing wind and diffusivity with their values at the source location, C''^{n} can be put in the form (for a general tri-dimensional situation):

$$C''^{n} = \frac{Q^{n-1/2}\,\Delta t}{8(\pi\Delta t)^{3/2} K_{x_s} K_{y_s} K_{z_s}} \exp\left\{ - \frac{(x - U_s\Delta t - x_s)^2}{4K_{x_s}\Delta t} - \frac{(y - V_s\Delta t - y_s)^2}{4K_{y_s}\Delta t} - \frac{(z - W_s\Delta t - z_s)^2}{4K_{z_s}\Delta t} \right\} \qquad (25)$$

if the additional assumption is that the boundaries have no effect on the dispersion of the puff for the time interval Δt*. (The subscript s in (25) indicates values taken at the source location (x_s, y_s, z_s).)

Equation (25) provides the contributions to be added to the grid points at every time step. Values given by (25) must be normalized to guarantee that at every time step the amount $\int_{(n-1)\Delta t}^{n\Delta t} Q(t')\,dt'$ is injected into the region.

Results from the application of the above algorithm are shown in Figures 5 and 6, which compare the root mean square of the deviations given by the finite difference scheme as applied in Figures 2 and 3 with that obtained by treating the source term as illustrated above. Figures 5 and 6 refer to a grid of (31 x 7) points and to a source located at $z_s = 0.5$ and 0.25 respectively. The reduction of ε_{mean} is greater for short simulation times and becomes negligible for long simulation times, thus confirming that errors in the treatment of the source term are smoothed out

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*Equation (25) can easily be modified to account for reflective boundaries.

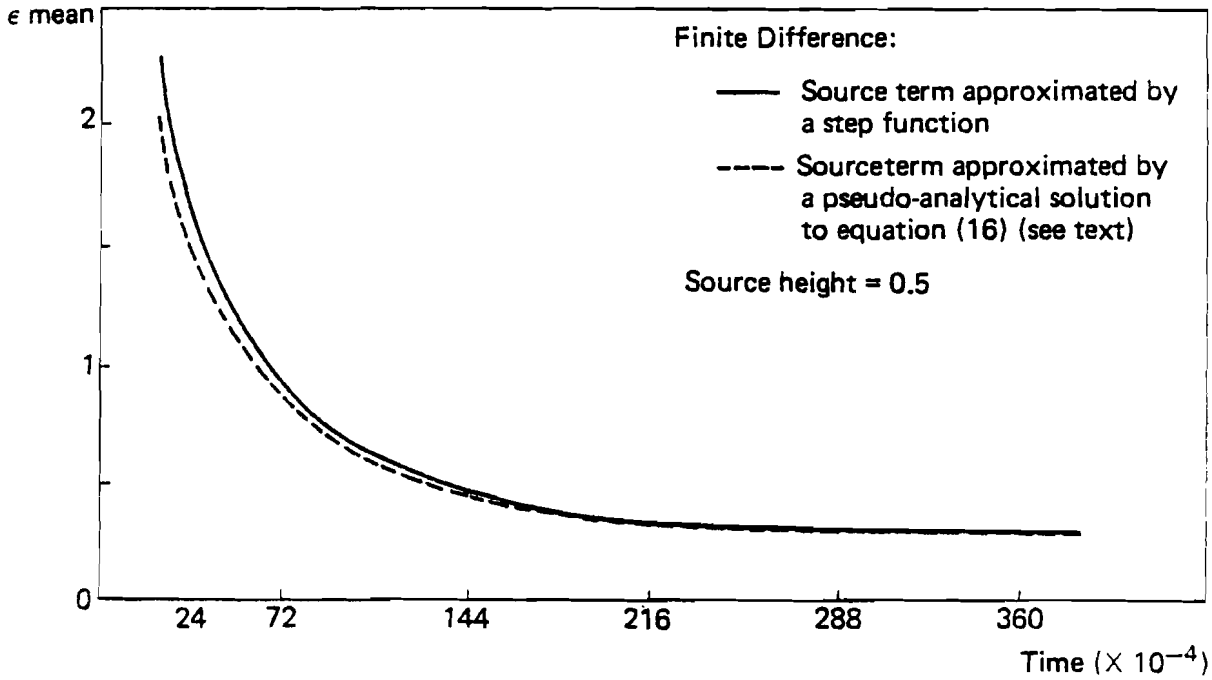

Figure 5. Comparison of ε_{mean} given by the finite difference (solid line) for a grid of (31 x 7) points and source height = 0.5 (same as in Figure 2) with the ε_{mean} achieved by treating the source item as proposed in the text (broken line).

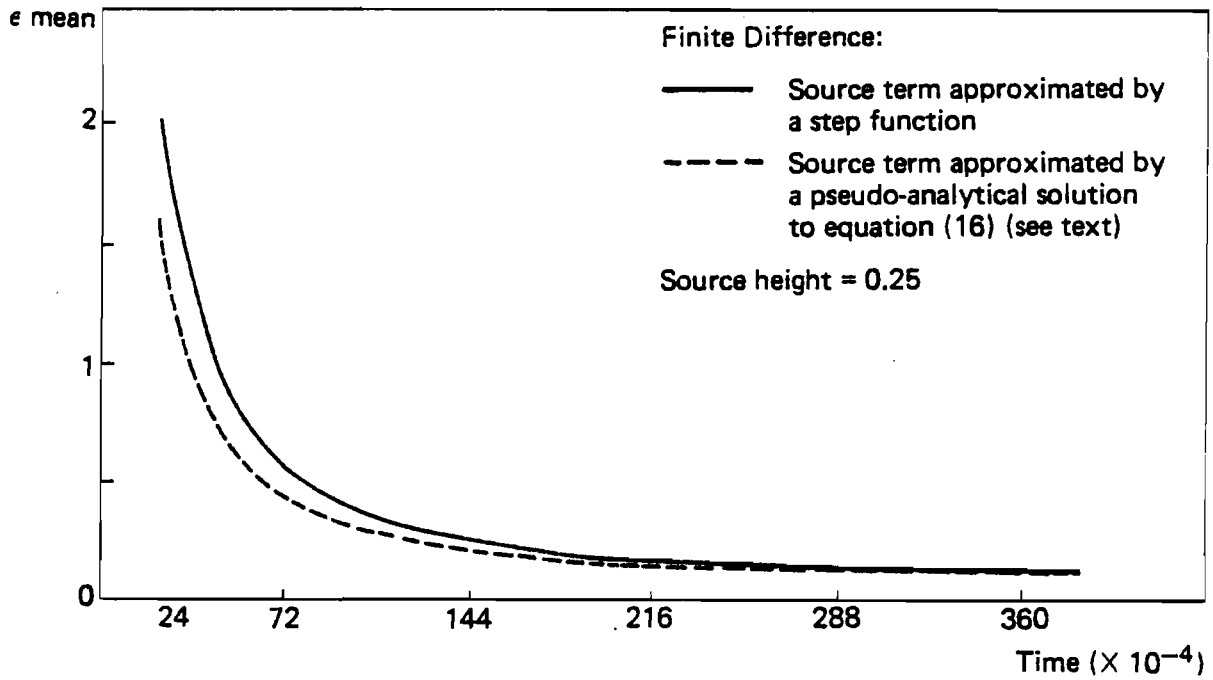

Figure 6. Same as for Figure 5, except that $z_s = 0.25$.

by the diffusion operator downwind of the source.

The proposed method rationalizes the treatment of the source term of (1). In other words, it describes the mathematically correct procedure to be followed in order to account for the source term in a finite difference algorithm. The errors introduced by the approximation of the contribution given by the instantaneous puff $Q^{n-1/2}\Delta t\ \delta(x_s - x)$ (see (16)) can be further reduced by looking for a more accurate solution than the one given by (25). However, improvement in the accuracy is primarily to be expected close to the source. The method can therefore substantially increase the accuracy of the solution in multiple source situations.

CONCLUSION

A finite difference and a Galerkin scheme are used in order to solve numerically a boundary value problem describing advection and diffusion of air pollutants from an elevated line source in an atmosphere vertically limited by an inversion layer.

Comparison of the results given by the two schemes with an accurate solution indicate that for both methods the grid spacing and integration time step cannot exceed the limits discussed in the text, in order to obtain a sufficiently accurate numerical solution, i.e., in order to avoid percent error much larger than 10% for significant values of the solution.

The Galerkin method describes better than the finite difference scheme the region close to the source for short simulation times. However, larger deviations in accuracy result from the Galerkin solution than from the finite difference scheme at points far from the source, particularly at the boundaries. The two

schemes prove equivalent for simulation time approaching the steady-state.

The errors presented by the finite difference scheme in points close to the source can be ascribed to the inaccurate estimation of the contribution given at every time step by the source term. By improving such an estimation deviation of the finite difference solution from the accurate one could be reduced. The proposed treatment of the source term by increasing the accuracy of the solution close to the source appears relevant to multiple source situations.

Considering that the Galerkin method requires more computer time, for cases similar to the one discussed in this study, the finite difference scheme is preferable. The Galerkin method, however, offers a valid alternative for those situations which require a complex grid geometry.

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