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A PRACTICAL NUMERICAL ALGORITHM TO
COMPUTE STEADY-STATE GROUND LEVEL
CONCENTRATION BY A K-MODEL

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PREFACE

Mathematical simulation of the dispersion and transformation processes undergone by the pollutants discharged into the atmosphere is fundamental to the evaluation of alternative strategies for the control and planning of emissions.

This paper is the first in a series in which mathematical modeling of air quality is discussed theoretically as well as in relation to application to real cases for both steady-state and time-dependent situations. It is expected that this series will contribute to rationalize and improve strategies for the protection of the atmospheric environment.

The present paper introduces a new algorithm to compute ground level concentrations of air pollutants for steady-state conditions. The proposed method which is built on the classical advection-diffusion continuity equation (named the K-model in this paper) improves the currently applied technique known as the Gaussian plume model.

ABSTRACT

A numerical algorithm to compute steady-state ground level concentration from elevated sources by means of a K-model which takes into account the spatial variability of wind and diffusivity and neglects horizontal diffusion is discussed. The boundary value problem to be treated, also for a point source, is always reduced to a two dimensional one and it is solved on an optimized grid. In this way the proposed method is made computationally comparable with the classical Gaussian plume model.

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E. Runca

1. INTRODUCTION

The most common way to compute ground level concentration from an elevated point source is based on the application of the following formula known as the Gaussian plume model:

$$C(x,y,o) = \frac{Q}{\pi \bar{U} \sigma_y(x) \sigma_z(x)} \exp \left\{ - \frac{y^2}{2 [\sigma_y(x)]^2} - \frac{h^2}{2 [\sigma_z(x)]^2} \right\} \quad (1)$$

In equation (1) the source is assumed to be located in the origin of the reference frame; the x-axis is chosen parallel to the wind direction; h is the plume axis (i.e. the stack height plus the plume rise); Q is the emission rate; \bar{U} is a representative value of the wind speed (in general it is the value of the wind speed at the height of the chimney); σ_y and σ_z are the standard deviations of the concentration distribution in the y and z directions, respectively.

Equation (1) is obtained under the assumptions (see, e.g. Seinfeld, 1975) that the turbulent diffusion process is stationary and homogeneous; the emission rate is constant; the horizontal diffusion is negligible with respect to advection; the ground

is a perfect reflector and the atmosphere is unbounded, i.e. no inversion is acting to suppress the vertical diffusion of the airborne matter, or at least, the ratio between the mixing height and the plume axis height is such that the influence of the inversion layer is felt quite far downwind from the source.

The Gaussian plume model was initially proposed by Sutton (1932), since then, in spite of the limiting assumption on which it is based, it has been extensively applied also to complex multiple source situations (see e.g. Turner 1964, Shieh et al. 1972; Runca et al. 1976).

Another way to model dispersion of air pollutants is provided by the classical advection-diffusion equation which for a point source of constant emission rate Q , assuming steady-state, wind horizontally uniform, negligible horizontal diffusion, and the reference frame defined as for equation (1) takes the form:

$$U(z) \frac{\partial C}{\partial x} = K_y(x, z) \frac{\partial^2 C}{\partial y^2} + \frac{\partial}{\partial z} \left(K_z(x, z) \frac{\partial C}{\partial z} \right) + Q \delta(x) \delta(y) \delta(z-h) \quad (2)$$

where K_y and K_z are the eddy diffusion coefficients (crosswind uniformity has been assumed) in the y and z directions, respectively, and $\delta(\bullet)$ is the Dirac's function. As for equation (1) the spatial resolution of equation (2) is limited by the Lagrangian length scale of the atmospheric turbulence. However, since equation (2) allows to take into account the spatial variation of wind and eddy diffusivity it provides a model more flexible than the Gaussian one. Limitations of K -models have been discussed, among others, by Lamb and Seinfeld (1973) and Corrsin (1974).

The Gaussian formula has been generally preferred to the K -model as it avoids the costs and the problems connected with the use of equation (2); specifically when the effects of different meteorological conditions and different source heights on the ground level concentration (to which air quality standards apply) have to be analyzed. With the Gaussian model, such analysis is computationally very simple, while the application of a K -model requires (the analytical solution, being in general, not available) the numerical integration of equation (2) on a tridimensional grid for each one of the considered cases. Hence, it

appears that in order to make the K-model as usable as the Gaussian one the integration of equation (2) has to be made inexpensive in terms of both programming and computer time.

This paper presents a practical method to compute ground level concentration by a K-model. First, the numerical algorithm is discussed for the two dimensional case describing dispersion from a crosswind infinite line source. Then, the proposed method is tested for a situation having an analytical solution and thereafter, it is applied to neutral stability conditions. Finally, extension of the method to three dimensions is discussed.

2. TWO-DIMENSIONAL MODEL

Assuming for the moment that the eddy diffusivity is only a function of the vertical coordinate, the concentration downwind from a line source is given by the solution to the following boundary value problem:

$$U(z) \frac{\partial C}{\partial x} = \frac{\partial}{\partial z} \left(K_z(z) \frac{\partial C}{\partial z} \right) + \delta(x) \delta(z-h) \quad (3)$$

$$K_z(z) \frac{\partial C}{\partial z} = 0, \quad z = 0 \quad (3a)$$

$$C(x, z) = 0, \quad z = \infty \quad (3b)$$

$$C(x, z) = 0, \quad x < 0; \quad x = \infty \quad (3c)$$

To generalize results given by the solution to equation (3) and related boundary conditions (3a)-(3c), x , z , C , U , and K_z have been expressed in units of $\frac{H^2 U(H)}{K_z(H)}$, H , $\frac{Q}{U(H)H}$, $U(H)$, and $K_z(H)$, respectively. In this way the source strength Q (see equation (3)) is normalized to one. H is a suitable vertical length scale, hereafter, taken as the height of the planetary boundary layer.

For the boundary value problem (3)-(3c), the reciprocal theorem (Smith 1957) gives:

$$C_h(x, 0) = C_0(x, h)$$

where $C_h(x,0)$ is the ground concentration due to a source of height h and $C_0(x,h)$ is the concentration at height h due to a ground level source.

By virtue of the above equation, the solution to the boundary value problem (3)-(3c), with the source located at ground level ($h=0$), allows one to derive the concentration at the ground for a source of any height. Thus, as generally happens, if the objective is the computation of the concentration at ground level as a function of the source height, equation (3) needs to be integrated for a given meteorological condition only for the case $h=0$. This obviously results in quite substantial saving of computer time and poses the only problem of defining a numerical algorithm to provide accurate solution to equation (3) for the case $h=0$.

Definition of this numerical algorithm has to deal with the following problems: (a) approximation of the δ -function representing the source term in equation (3) and (b) approximation of the boundary condition (3b).

Approximation of the δ -function, as already proposed by Melli and Runca (1979), can be achieved by finding an approximate analytical solution to the boundary value problem (3)-(3c) in a region close to the source. Such approximate solution is used to estimate the concentration profile in a downwind section (located at a suitable distance x_b from the source) which is then taken as the left boundary of the integration region. Application of this procedure is discussed further later.

More complex in some way is the definition of the upper boundary of the integration region. Let us call z_s the height of the upper boundary and for the moment, let us assume it constant. Since condition (3b) has to be approximately verified at every point downwind from the source, z_s is determined by the right extreme (the farthest downwind point) of the integration region, as this is the point at which pollutant particles have spread to the maximum height. At the right extreme, the vertical concentration profile is quite smooth (assuming that this point is sufficiently far from the source) and can be described by a limited number of grid points uniformly spaced. Going backward

towards the source, the concentration profile gets steeper and pollution is confined to layers close to the ground. To describe this situation, being z_s constant, either the number of grid points has to be increased in the vertical sections close to the source or the grid points have to be unevenly spaced in such a way to have more points close to the ground where the concentration gradients are larger. Both these two approaches do not look convenient. The increase of the grid points number means increase of memory and computer time, the disuniform distribution of grid points can create close to the source too much large differences in the grid spacing and consequently, possible reduction of the accuracy of the numerical solution.

From the above considerations it seems more appropriate not to keep z_s constant, but to consider it a function of the downwind distance from the source by defining it as the level at which in every section the concentration becomes negligible. With this choice, assuming that z_s is known and considering, for the sake of simplicity, uniform spacing, both in the vertical and in the horizontal, the integration grid appears as in Figure 1. Use of an upper boundary function of x clearly allows one to describe accurately the concentration profile in every downwind section with the same number of points. This approach, as Figure 1 illustrates, requires that the numerical integration be done on an irregular grid. However, we will show below that due to the type of the problem described by equation (3)-(3c), a standard finite difference scheme can be applied to the grid of Figure 1.

3. NUMERICAL ALGORITHM

Considering the possibility of using disuniform grid spacing, both in the horizontal and in the vertical, the Crank-Nicolson scheme (see e.g. Richtmyer and Morton 1967) has been applied to equation (3), yielding the finite difference equation:

$$C_{i,k} = C_{i-1,k} + \frac{\Delta x_{i-1}}{\bar{U}_k \Delta z_k (\Delta z_{k-1} + \Delta z_k)} \left\{ D[C_{i,k}] + D[C_{i-1,k}] \right\} \quad (4)$$

with

$$\bar{U}_k = \frac{2}{\Delta z_{k-1} + \Delta z_k} \int_{z_{k-1} + \frac{\Delta z_{k-1}}{2}}^{z_k + \frac{\Delta z_k}{2}} U(z) dz$$

and

$$D[C_k] = K_{k+\frac{1}{2}} C_{k+1} - \left(K_{k+\frac{1}{2}} + \frac{\Delta z_k}{\Delta z_{k-1}} K_{k-\frac{1}{2}} \right) C_k + \frac{\Delta z_k}{\Delta z_{k-1}} K_{k-\frac{1}{2}} C_{k-1}$$

In equation (4) Δx_{i-1} is the horizontal interval between points $i-1$ and i , Δz_k is the vertical interval between points k and $k+1$, and N is the number of points in every section.

The immediate consideration arising from the analysis of equation (4) is that, in order to compute the concentration in the i^{th} section, the concentration values in the $i-1^{th}$ section have to be known at the same levels of the grid points of the i^{th} section. This is obviously not the case for the grid reported in Figure 1. However, assuming that the concentration is known at the $i-1^{th}$ section, the concentration values at the levels corresponding to the points of i^{th} section can be determined by an interpolation algorithm. Due to the definition of z_s to the concentration in the points falling at or above z_s is assigned the value zero. The situation is illustrated in Figure 2.

In the application of this algorithm the condition to be fulfilled in every section is:

$$\int_0^{z_s(x)} U(z) C(x, z) dz = 1 \quad (5)$$

The finite difference analog to equation (5) has the form:

$$\sum_{k=1}^N U_k C_{i,k} \frac{\Delta z_{k-1} + \Delta z_k}{2} = 1 \quad (6)$$

Equation (6) must not be violated when the profile concentration in the $i-1^{th}$ section is described by the interpolated points. This implies (see Figure 2) that accuracy is not lost when the grid spacing is changed in $i-1^{th}$ section from the value $(\Delta z)_{i-1} = \frac{z_s(x_{i-1})}{N-1}$ to the value $(\Delta z)_i = \frac{z_s(x_i)}{N-1}$. In other words, the number of grid points N must be chosen in such a way that in the $i-1^{th}$ section the true

concentration profile can be approximated by a piecewise linear function described by N values distributed once on the interval $0-z_s(x_{i-1})$ and once on the interval $0-z_s(x_i)$. Achievement of this condition, given N , depends on Δx_{i-1} and on $\frac{dz_s}{dx}$. Since the highest growth rate of z_s occurs close to the source, small values of Δx are required close to the source. Thus the use of uniform horizontal grid spacing is not very convenient as it can require a very large number of points to describe the integration region. An horizontal grid spacing increasing with the distance from the source is then more suitable, as it will be shown later to the application of the above described numerical procedure.

Considering that the largest concentration gradient occurs at the ground, it seems convenient to use, also in the vertical, not a uniform grid spacing; specifically a vertical grid size increasing with the distance from the ground. However, in the tests performed, a variable vertical grid spacing did not give the same increase in accuracy like the use of variable horizontal grid spacing. The improvement due to a more appropriate distribution of the points in the vertical was probably counterbalanced by the decrease of the order of the truncation error of the Crank-Nicolson scheme from Δz^2 to Δz , which occurs when disuniform spacing is used.

Up to now the choice of N and its relation with z_s has not been explained. Analysis of equation (4) indicates that concentration in the i^{th} section depends only on the i^{th} section. Thus, the "key-section" in the application of this algorithm is the one at $x = x_b$. Assuming that z_s is known, N must be such that the concentration profile can be described by a piecewise linear function in this section.

Estimation of the concentration profile at $x = x_b$ implies the approximation of the source term of equation (3). This is discussed below.

3.1 Source term approximation

The simplest way to approximate the source term is the replacement of the δ -function with a step function in such a way that equation (6) is satisfied. This approach for a source

located at ground introduces very large errors as the wind speed is zero at the source level. In addition, the representation of the δ -function by a step function implies that some diffusion of the pollutant matter has occurred. Thus the step function has to be located at some undefined downwind distance. To give a better representation of the δ -function term of equation (3), the method proposed by Melli and Runca (1979) can be used.

This method is based on the concept that in the region close to the source diffusion of pollutants depends substantially on wind and diffusivity values close to the source. This suggests to replace in equation (3) the wind and diffusivity with approximating functions which maintaining the basic characteristics of the wind and diffusivity close to the source allow at the same time the derivation of an analytical solution to equation (3). Such analytical solution can then be assumed as an approximation of the true concentration distribution in the region close to the source and used to compute the concentration profile at $x = x_b$. The analytical solution at $x = x_b$ is then approximated by a piecewise linear function over N points chosen in such a way that equation (6) is satisfied. The quote $z_s(x_b)$ is the one at which concentration is approximately zero. Computation of z_s is discussed below.

3.2 Definition of the upper boundary

Once $z_s(x_b)$ is defined by taking it as the level at which the concentration is approximately zero, the ratio $\gamma = C_{z_s}/C_{z=0}$ is known at section $x = x_b$. The profile z_s can then be computed under the assumption that γ be the same in every section. Computation of z_s is obviously trivial should the problem (3) - (3c) have an analytical solution. In the general case z_s has to be determined by means of some approximate solution which guarantees an overestimate of it, as it is shown in the example reported below.

Verification of the method in a case for which the boundary value problem (3)-(3c) has an analytical solution as well as application to a situation representative of neutral atmospheric stability is now discussed.

4. VERIFICATION AND APPLICATION

For wind and diffusivity expressed by $U = z^\alpha$ and $K_z = z^\beta$, respectively, the solution to the boundary value problem (3) - (3c), with $h = 0$, is (see Smith 1957):

$$C_0(x, z) = \frac{\alpha-\beta+2}{\Gamma(s)} \left[\frac{1}{(\alpha-\beta+2)^2 x} \right]^s \exp \left[- \frac{z^{\alpha-\beta+2}}{(\alpha-\beta+2)^2 x} \right] \quad (7)$$

where $s = (\alpha+1)/(\alpha-\beta+2)$ and $\alpha-\beta+2 > 0$.

Defining z_s as the height at which $C_0(x, z_s) = \gamma C_0(x, 0)$ equation (7) gives:

$$z_s = \left[(\alpha-\beta+2)^2 x \log \frac{1}{\gamma} \right]^{\frac{1}{\alpha-\beta+2}} \quad (8)$$

With the above defined z_s , first, equation (3) has been integrated in the rectangular region ($0 \leq x \leq 0.15$, $0 \leq z \leq z_s(x=0.15)$) by distributing uniformly M points in the horizontal and N points in the vertical. Successively it has been integrated over the same number of points allowing z_s to change with x according to equation (8). In this computation Δz changes with x and is kept uniform in every vertical section (see Figure 1). Finally, equation (3) has been integrated over the same number of points by taking z_s function of x and by using both in the horizontal and in the vertical a variable grid spacing.

The computations utilized for figures 3 and 4, which will be illustrated below, refer to $\alpha = 0.15$ and $\beta = 1$ and were done with $M = 151$ and $N = 121$. Equation (7) provided the concentration profile at $x = x_b$, which was taken equal to Δx_1 . In defining the geometry of the integration grid N must be chosen in such a way that the constant flux condition (equation (6)) is verified also by the concentration profile obtained after the application of the interpolation procedure.* This implies that N must be

* Rescaling of the concentration values, in order to verify equation (6), is only allowed at $x = x_b$.

sufficiently large. In the tests performed, equation (6) was always accurately approximated at 121 points. Satisfactory approximation was also achieved at 80 points. However, results here are reported for $N = 121$ in order to show that even in the case of a relatively refined uniform grid an upper variable boundary produces a remarkable increase in the accuracy of the numerical solution. Such an increase is more pronounced with course grids.

Figure 3 displays the percent error computed in every vertical section by comparison with the analytical solution (equation (7)) at the point where the maximum absolute error was found. The error is reported both for $z_s = \text{const}$ and $z_s = f(x)$ as given by equation (8) with $\gamma = 10^{-9}$. Use of z_s function of x reduces the error of one order of magnitude. Further reduction of the error is achieved by taking $\Delta x = f(x)$ and $\Delta z = f(z)$ as shown in Figure 4. The plots of Figure 4 were obtained by defining both Δx_1 and $\Delta z_{i,1}$ equal to one-tenth of their respective values corresponding to the uniform grid spacing distribution. The successive values of Δx and Δz_i were then increased in such a way to reach with 150 and 120 intervals respectively the horizontal coordinate $x = 0.15$ and the vertical coordinate $z_i = z_s(x_i)$. The plot of Figure 4 indicates that the accuracy of the results depends strongly on the geometry of the grid. However, this point is here not further investigated. More relevant is the application of the proposed algorithm to the general case in which the analytical solution to the boundary value problem (3) - (3c) is unknown. This is described in the following with reference to dispersion in a neutral atmosphere.

Both theoretical (see, e.g. Shir, 1973; Wyngaard et al, 1974) and experimental work (Robins, 1978) have shown that the neutral vertical eddy diffusivity profile can be represented by an exponential law, which, following Shir and Shieh (1974) can be expressed in normalized units by the function:

$$K_z = z e^{-\rho(z-1)} \quad (9)$$

In equation (9) ρ is a dimensionless parameter (approximately equal to 4 for neutral conditions) whose reciprocal gives the fraction of the height of the planetary boundary layer at which the maximum value of K_z occurs.

With $U = z^\alpha$ and K_z given by relation (9) equation (3) takes the form:

$$z^\alpha \frac{\partial C}{\partial x} = \frac{\partial}{\partial z} \left(z e^{-\rho(z-1)} \frac{\partial C}{\partial z} \right) + \delta(x) \delta(z) \quad (10)$$

Straightforward analysis of equation (10) shows that the concentration close to the source can be approximated by the solution to the equation:

$$z^\alpha \frac{\partial C}{\partial x} = \frac{\partial}{\partial z} \left(z e^\rho \frac{\partial C}{\partial z} \right) + \delta(x) \delta(z) \quad (11)$$

obtained by replacing in equation (10) the vertical eddy diffusivity profile with its tangent in the origin. Considering the scaling factor e^ρ and noticing that $\beta = 1$ the solution to equation (11) is derived from equation (7) in the form:

$$C = \frac{e^{-\rho}}{(1+\alpha)x} \exp \left[- \frac{z^{1+\alpha} e^{-\rho}}{(1+\alpha)^2 x} \right] \quad (12)$$

Equation (12) provides the required approximation of the concentration profile at $x = x_b$. In this way no arbitrary approximation of the source term has to be done for the application of the finite difference equation (4).

Equation (12) can be also used to provide the estimation of the upper boundary z_s . This stems immediately from the comparison of equation (10) with (11). Being $K_z = z \exp(\rho)$ greater than $K_z = z \exp[-z(\rho-1)]$ at any level, equation (11) describes a process in which the material diffuses faster, and therefore to higher levels, than in the situation described by equation (10). Hence equation (12) guarantees an over-estimate of z_s .

It is expected that, in the majority of the cases, it should be possible, by proceeding in a way similar to the example discussed above, to determine for the boundary value problem (3) - (3c) both an approximation of the concentration in the region close to the source and an estimate of the upper boundary $z_s(x)$ of the integration region. With this assumption the method acquires a general applicability. Its computational efficiency is apparent in a multiple source situation. In fact, said (x_k, h_k) the location and the effective height of the k^{th} -source, respectively, the concentration at the ground due to N_s -sources is simply given, for a given meteorological condition, by:

$$C(x, 0) = \sum_{k=1}^{N_s} C_0(x - x_k, h_k) \quad (13)$$

with $C_0(x - x_k, h_k) = 0$ for $(x - x_k) \leq 0$.

In equation (13) the concentration C_0 is the matrix given by the numerical integration of equation (3) with $h = 0$. Simple interpolation procedures are used for the $(x - x_k, h_k)$ locations which do not follow in the points of the grid.

Since the reciprocal theorem proved by Smith (1957) does not depend on the functional form of the diffusion coefficients the proposed method and the related equation (13) hold also for diffusivity profiles which are a function of the downwind distance from the source. However, for the sake of completeness, we recall that if the diffusivity profile can be expressed as:

$$K_z = f(x)g(z) \quad (14)$$

the definition of the new variable (see also Csanady, 1973):

$$\xi = \int_0^x f(x') dx' \quad (15)$$

reduces the problem to the one described by equation (3)-(3c), in which x and K_z are respectively replaced by ξ and $g(z)$.

5. THREE-DIMENSIONAL MODEL

Extension of the proposed method to the three dimensional situation described by equation (2) with boundary conditions similar to the ones given by the relations (3a)-(3c) has no specific limitation. The equivalent of equation (13) is:

$$C(x, y, 0) = \sum_{k=1}^{N_s} C_0(x-x_k, y-y_k, h_k) \quad (16)$$

However, two difficulties arise. The first one concerns the loss of computational efficiency with respect to the two dimensional case. The second one derives from the fact that for equation (2), even in the case of U , K_y and K_z expressed by power law of the vertical coordinate, an analytical solution is generally not available, thus making problematic both the approximation of the source term and the estimation of z_s .

Both the problems mentioned above can be solved if it is assumed that the concentration profile in the y direction is gaussian. This assumption which was proposed by Smith (1957) (see also Demuth and Berger 1977) is suggested by the way in which y variations appear in equation (2). There are also experimental evidences that the crosswind concentration distribution is approximately Gaussian. On this basis the solution to equation (2) for a ground level source can be assumed to have the form:

$$C_0(x, y, z) = x_0(x, z) \cdot \frac{e^{-\frac{y^2}{2[\sigma_y(x, z)]^2}}}{\sqrt{2\pi} \sigma_y(x, z)} \quad (17)$$

Defining the following moments of the concentration distribution:

$$C_{00} = \int_{-\infty}^{+\infty} C_0 dy \text{ and } C_{02} = \int_{-\infty}^{+\infty} y^2 C_0 dy$$

it is immediately seen that $C_{00} \equiv x_0(x, z)$ is the solution to the two dimensional boundary-value problem (3)-(3c) while

$$\sigma_y(x, z) = \left(\frac{C_{02}}{C_{00}} \right)^{\frac{1}{2}} \quad (18)$$

Use of equation (17) reduces the tri-dimensional problem to the two dimensional one. Equation (16) can be replaced by the most convenient expression:

$$C(x, y, 0) = \sum_{k=1}^N x_0(x-x_k, h_k) \frac{e^{-\frac{(y-y_k)^2}{2[\sigma_y(x-x_k, h_k)]^2}}}{\sqrt{2\pi} \sigma_y(x-x_k, h_k)} \quad (19)$$

However, use of equation (19) implies the knowledge of $\sigma_y(x, z)$, which is given by equation (18). Hence, C_{02} has to be determined; this involves the solution of the following boundary value problem:

$$U \frac{\partial C_{02}}{\partial x} = \frac{\partial}{\partial z} \left(K_z \frac{\partial C_{02}}{\partial x} \right) + 2 K_y C_{00} \quad (20)$$

$$K_z \frac{\partial C_{02}}{\partial z} = 0, \quad z = 0 \quad (20a)$$

$$C_{02}(x, z) = 0, \quad z = \infty \quad (20b)$$

$$C_{02}(x, z) = 0, \quad x = 0; x = \infty \quad (20c)$$

In deriving equation (20) use has been made of the Dirac's function property:

$$\int_{-\infty}^{+\infty} f(y) \delta(y-y_0) dy = f(y_0)$$

The solution of equation (20) with the related boundary conditions presents no difficulty. The same grid adopted for computing C_{00} and a modified equation (4) to take into account the forcing term ($2K_y C_{00}$) can be used to integrate the boundary value problem (20)-(20c). Large errors occur at the upper boundary z_s where both C_{00} and C_{02} go to zero. The evaluation of σ_y cannot therefore be extended up to z_s ; the computation must terminate few grid points below z_s .

With the above formulation the tri-dimensional case is reduced to the solution of two bi-dimensional problems. For the sake of completeness, it must be added that for the special case of lateral diffusivity having the form

$$K_y = f(x)U(z) \quad (21)$$

equation (20) has the simple solution

$$C_{02} = 2 C_{00} \int_0^x f(x') dx'$$

Thus, for those circumstances in which equation (21) holds the tri-dimensional problem is computationally equivalent to the bi-dimensional one.

6. CONCLUSION

Use of the reciprocal theorem proved by Smith (1957) and the definition of a simple finite difference algorithm have made possible the computation of steady-state ground level concentration downwind of both single and multiple source situations by a K-model without any loss of computational efficiency in comparison with the classical Gaussian plume model.

The proposed method requires also in a point source situation the solution of only bi-dimensional boundary value problems. It can therefore be programmed on a very small computer and is suitable to interactive languages, in this way providing the user with the capability to analyze in a very straightforward manner concentration profiles due to different source distributions as well as effects of grid geometry and parameters on the solution.

It is well known that K-theory provides only an approximate description of the processes which affect atmospheric diffusion. For those situations in which K-theory can be applied the proposed method can replace the Gaussian plume model. At more or less the same cost it provides the user with the possibility to analyze the effect on the steady-state ground level concentration of wind and diffusivity spatial variability, both in single and multiple source situations.

REFERENCES

- Corrsin S. (1974) Limitations of gradient transport models in random walks and in turbulence. Adv. Geoph. 18A, Wiley-Interscience. 25-60.
- Csanady G.T. (1973) Turbulent diffusion in the environment. D. Reidel Publishing Company, Dordrecht-Holland.
- Demuth C. and Berger A. (1977) Evaluation de la pollution à l'aide d'un modèle à coefficient de diffusion variables. Scientific Report AL/1/4.1.5, National R-D Program on Environment-Air, Services for Science Policy Programming, Belgium.
- Lamb R.G. and Seinfeld J.H. (1973) Mathematical modeling of urban air pollution. Environmental Science & Technology 7, 253-261.
- Melli P. and Runca E. (1979) Gaussian plume model parameters for ground-level and elevated sources derived from the atmospheric diffusion equation in a neutral case. J. Appl. Meteor. 18, 1216-1221.
- Richtmyer R.D. and Morton K.W. (1967) Difference methods for initial-value problems. Interscience, New York.
- Robins A.G. (1978) Plume dispersion from ground level sources in simulated atmospheric boundary layers. Atmos. Environm. 12, 1021-1032.
- Runca E., Melli P. and Zannetti P. (1976) Computation of long-term average SO₂ concentration in the Venetian area. Appl. Math. Mod. 1, 9-15.
- Seinfeld J.H. (1975) Air pollution: physical and chemical fundamentals. McGraw-Hill, New York.
- Shieh L.H., Halpern P.K., Clemens B.A., Wang H.H. and Abraham F.F. (1972) Air quality diffusion model: application to New York City. IBM J. Res. Develop. 16, 162-170.
- Shir C.C. (1973) A preliminary numerical study of atmospheric turbulent flows in the idealized planetary boundary layer. J. Atmos. Sci. 30, 1327 - 1339.
- Shir C.C. and Shieh L.H. (1974) A generalized urban air pollution model and its application to the study of SO₂ distributions in the St. Louis Metropolitan Area. J. Appl. Meteor 13, 185-204.
- Smith F.B. (1957) The diffusion of smoke from a continuous elevated point source into a turbulent atmosphere. J. Fluid. Mech. 2, 49-76.

- Sutton O.G. (1932) A theory of eddy diffusion in the atmosphere.
Proc. Roy. Soc. (London) A 135, 143-165.
- Turner D.B. (1964) A diffusion model for an urban area.
J. Appl. Meteor. 3, 83-91.
- Wynngaard J.C., Coté O.R. and Rao K.S. (1974) Modeling the
atmospheric boundary layer. Adv. Geoph. 18A, Wiley-
Interscience, 193-212.

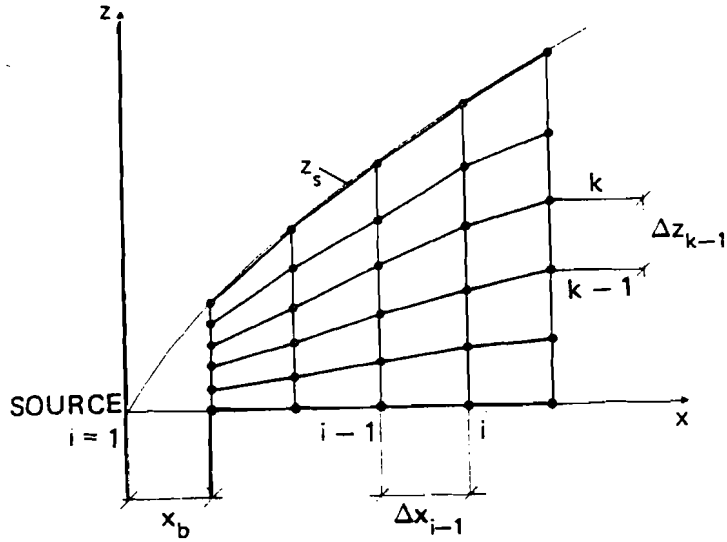


Figure 1 - Integration grid geometry with both horizontal and vertical uniform spacing. z_s is the level at which the concentration becomes negligible (i.e. a very small fraction of the ground level concentration); x_b is the location of the section where the vertical concentration profile is determined analytically.

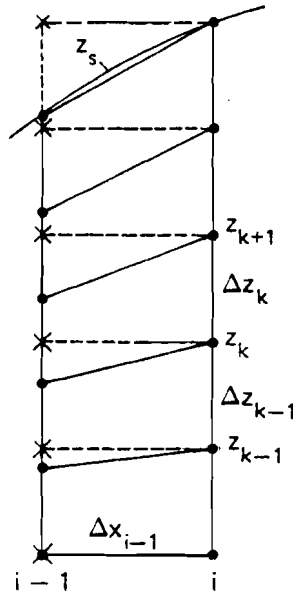


Figure 2 - Illustration of the application of the finite difference equation (4) (see text) to the grid of Figure 1. X indicates the points of section (i-1) corresponding to the points of section i. At these points the concentration is estimated by a linear interpolation.

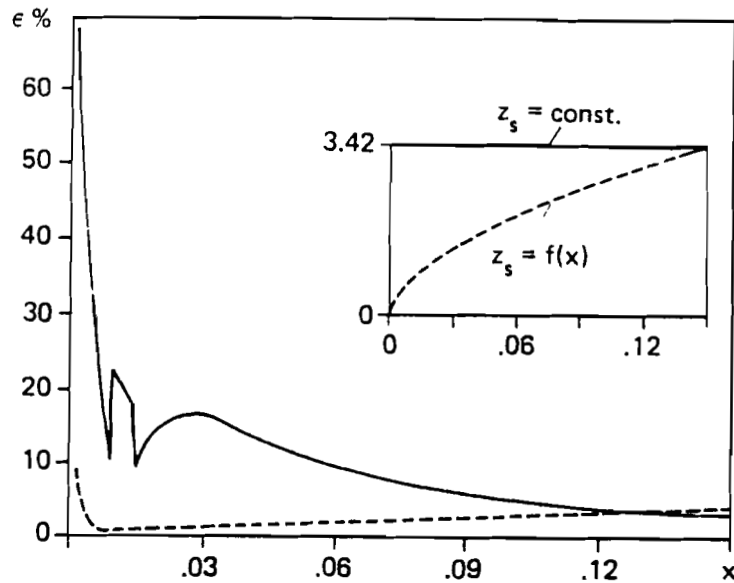


Figure 3 - Comparison of analytical and numerical solution. The plots represent the per cent error recorded in every vertical section in the location where the maximum absolute error occurred. The solid line refers to a constant upper boundary, the dashed one to an upper boundary function of the downwind distance (i.e. to a grid geometry as in Figure 1).

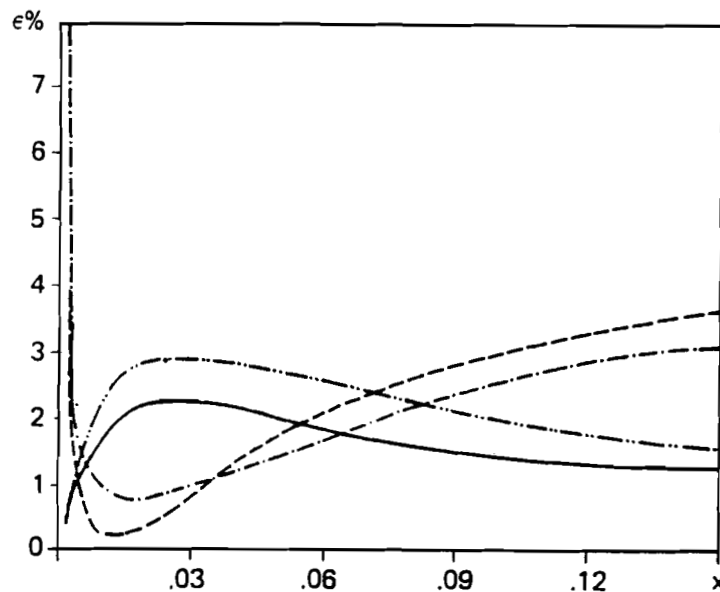


Figure 4 - Comparison of analytical and numerical solution. The plots represent the per cent error as defined in Figure 3 for an upper boundary function of the downwind distance. The different lines refer to: ---- Δx and Δz uniform (same as in Figure 3); -.-.- Δx uniform and $\Delta z = f(z)$; -.-.-.- $\Delta x = f(x)$ and Δz uniform; ——— $\Delta x = f(x)$ and $\Delta z = f(z)$.