TOWARDS MAKING ADVECTION-DIFFUSION SOLVERS AS FAST AS GAUSSIAN ONES: A PROPOSAL FOR ATMOSPHERIC POLLUTION

Carlos López Vázquez

Centro de Cálculo
Facultad de Ingeniería. Montevideo (Uruguay)
carlos@fing.edu.uy

ABSTRACT:

Based on the K-model, an alternative solution to the problem of forecasting atmospheric pollution other than the Gaussian models (either the plume or the puff) is presented. It is intended to show its possible use for the long-term as well as for the real-time forecast. My proposed procedure is expected to take similar computer time to Gaussian models, thereby eliminating the main objection for its use.

Key word index: advection-diffusion solver, atmospheric diffusion, real-time forecast, air pollution

1. INTRODUCTION:

It is well known that the Gaussian models have been and still are of widespread use in the analysis of the advection of pollutants. The main advantage of Gaussian models is that they are simple and economical as far as computer-time is concerned. These advantages enable the user to address long-term as well as real-time forecasts. A comprehensive literature dealing with the determination and measurement of the parameters σ_z and σ_y of the Gaussian plume model has accumulated for a wide range of cases.

In fact, it is common practice in the U.S. to use models derived from the Gaussian law.
However, as the Gaussian models cannot easily deal with chemical reactions, ground deposition, rainwash, etc., a great effort has been made to develop other methodologies, particularly the one based on the K-model, which will be referred to in the present work.
The K-theory, or first order closure model, has been widely used in theoretical studies with simple shapes. In fact, this theory is hardly ever used in the case of multiple and irregularly distributed sources, as is the case in cities, for examples. As an exception to this rule, Reynolds, Roth and Seinfeld, 1973, modeled the airshed of Los Angeles using the K-theory. In this particular case, eight computer hours on an IBM 370/155 were required to calculate the pollutant field for an hour. Undoubtedly, hardware advances have reduced computer costs, but calculations based on the K-theory still remain at a disadvantage as to computer time costs in comparison to the algebraic formulations characteristic of the Gaussian models. Therefore, in this work, a methodology is presented which permits lowering computation costs to a level comparable of the Gaussian models.

2. OVERALL FORMULATION OF THE MODEL

I will refer to the case of a single pollutant, which is advected by a given windfield, assumed to be steady for the interval $[t,t+\Delta t]$. A gravitational settling velocity, an exponential rate decay and a ground level absorption or emission can all be attributed to the pollutant.
The above can be modeled according to the following general equation:

$$\frac{\partial C}{\partial t} + \bar{v}.\nabla C - \nabla(\mathbf{K}.\nabla C) - W_D.(\bar{n}.\nabla C) - \Lambda.C = \sum_i S_i(X,Y,Z,t) \quad \textbf{(1)}$$

Where:

C : Concentration of the pollutant (kg/m)

$\bar{v} = (u, v, w)$: Time dependent windfield (three components) (m/s)

$$\mathbf{K} = \begin{bmatrix} K_H & 0 & 0 \\ 0 & K_H & 0 \\ 0 & 0 & K_V \end{bmatrix}$$

being K_H : Horizontal eddy viscosity coefficient (m / s)
K_V : Vertical eddy viscosity coefficient (m / s)

Λ : Generation or decay rate of the pollutant (1/s)

S_i : Point source of pollutant (kg/m /s)

W_D : Gravitational settling of the pollutant (is positive downwards) (m/s)

X,Y,Z : Coordinates in an absolute reference system (Eulerian)

Equation (1) can be solved subject to the proper boundary conditions (BC). I shall assume that the domain can be divided into zones where the windfield is locally unidirectional for the interval [t,t+Δt]. Then, the problem can be reformulated choosing a system of coordinates in such a way that the axis Ox is in the direction of the horizontal wind. Such system is valid only for the interval [t,t+Δt].

Taking this into consideration, I shall show that being (1) a linear equation, it is possible to obtain a result for field C(x,y,z,t+Δt), by means of a linear combination of previously calculated results. Thus, the field of the pollutant in the whole workspace can be considered as a superimposition of the field calculated under unidirectional wind (but not necessarily uniform)

We will neglect topography, as well as nonlinear chemistry, and also assume that parameters

$\Lambda, W_D, K_H, K_V, V_D$ have values that are not a function of travel distance to the sources; i.e., we state that those parameters are only function of height z above ground, so they are independent of x, y. However, they can vary with time. This hypothesis will be discussed later.

In order to solve the problem, I shall point out two particular cases among the general case:

I) The case of the equation without sources

II) The case of the homogeneous initial condition with sources

I) The case of the equation without sources

The use of puff models for the simulation of the problem of advection of pollutants is extremely widespread. (See Ludwig et al, 1977, Ludwig, 1984, Sheih, 1978, etc.). The idea is based on the fact that if two or more puffs exist in t, the pollutant field in t + Δt may be calculated as a superimposition of the corresponding fields as if each puff were considered separately. This assumption precludes nonlinear chemistry effects. I shall put forth a similar idea at this point. According to common practice, in the following lines, I shall develop the definition of the pollutant fields by means of its value on the nodes of a pre-established regular grid (with Δx=Δy). The initial conditions as well as the final results can be defined through a finite number of values. If it is possible to express the initial condition in the following way:

$$C_0(x,y,z,t) = \sum_{l,m,n}^{L,M,N} C_{lmn}(t).H_{lmn}(x,y,z,0) \quad \textbf{(2)}$$

then, it may be observed that:

$C_{lmn}(t)$: is a weight coefficient, related to a reference concentration.

l,m,n : are the indexes corresponding to the grid values in direction x,y,z.

$H_{lmn}(x,y,z,0)$ is a shape function, which will be defined later.

Field $C(x,y,z,t+\Delta t)$ resulting from the resolution of equation (1), constrained by the BC, plus the initial condition (2), may be calculated as

$$C(x,y,z,t+\Delta t) = \sum_{l,m,n}^{L,M,N} C_{lmn}(t).H_{lmn}(x,y,z,\Delta y)$$

(3)

$H_{lmn}(x,y,z,\Delta t)$ is the result of solving (1)+BC, with the initial condition

$$C_0(x,y,z,t) = 1.H_{lmn}(x,y,z,0) \qquad \textbf{(4)}$$

The shape functions H_{lmn} (x,y,z,0) cannot arbitrarily be chosen, because they must fulfill identically the boundary conditions.

For the choice of such functions, I shall refer to a subset of continuous functions defined on the nodes of a grid. We will not use standard piecewise linear functions, in order to allow some manipulations which will be clearer later. We will require from the basis function the property of symmetry with respect the azimuth angle, so in polar coordinates, its shape depends only on distance from the point (x_l,y_m). Therefore, a suitable base to describe the initial condition may have basis functions that look like a cylindrical cone with $(x_l,y_m,1)$ as vertex coordinates, and the circle with center (x_l,y_m) and unit radii as a base. Such function can be precisely defined as

$$H_{lmn}(x,y,z,0) = F_{lm}(\rho).G_n(z), \qquad \text{being:}$$

$$F_{lm}(\rho) = F_{lm}\left(\sqrt{(x-x_l)^2+(y-y_m)^2}\right) = \begin{cases} 0 & \textit{if } \rho > \Delta x \\ 1-\dfrac{\rho}{\Delta x} & \textit{if } \rho \le \Delta x \end{cases}$$

and assuming $\Delta x=\Delta y$ hereinafter. Any other basis functions which are continuous, only function of ρ, which evaluate as 1 if $(x_i,y_j)=(x_l,y_m)$, and 0 elsewhere can be used instead. Notice that with this definition we obtain a set which is an orthogonal basis for the grid space. However, a constant pollution field cannot be represented exactly within grid values. Similarly $G_n(z)$ can be defined in order to verify identically BC at z=H or z=0.

Thus, it is observed that if the case of the homogeneous equation (without sources) (1) is considered, then, none of the terms depends on the absolute value of x or y; the parameters are only a function of z. Therefore, the evolution of a puff of the $C_{lmn}(t)H_{lmn}(x,y,z,0)$ type, with a center (x_l,y_m,z_n) only depends on the height z_n and not on the value of the coordinates (x_l,y_m). This assumption precludes consider topography.

Ensuingly, it is possible to calculate a catalogue of fields $H_{lmn}(x,y,z,\Delta t)$, after solving (1)+BC, and using as initial condition as many functions $H_{lmn}(x,y,z,0)$ as levels n are specified in the workspace. It should be pointed out that the functional shape of H_{lmn} at the time Δt is not imposed, unlike what would occur at the time 0. Instead, it results by solving the problem defined by (1),(4)+BC. The evolution of any puff, which can be calculated by solving the equation (1)+BC can be obtained as the linear combination of said fields $H_{lmn}(x,y,z,\Delta t)$, which have been calculated and previously stored. The costs in terms of computer time is minimal, once the $H_{lmn}(x,y,z,\Delta t)$ have been generated. This time consuming operation is performed only once.

Irrespective of the way used in calculating $H_{lmn}(x,y,z,\Delta t)$ its shape will not be stored as point values defined on a regular grid. Instead, it will be defined using two-dimensional Bezier curves, which are based upon control points (see Foley et al., 1990). This representation is independent from the underlying coordinate system, in opposition to polynomial, spline and similar alternatives. The reason for this uncommon approach will be evident in the next paragraph.

To sum up, what has been presented is a way of calculating the evolution of any puff initially existent at the time t, until the time t+Δt.

AN OUTLINE OF THE NUMERICAL PROCEDURE

Given an initial field at time t, $P_1(X,Y,Z,t)$, advected by a locally unidirectional windfield, it is intended to find $P_1(X,Y,Z,t+\Delta t)$ through the solution of the problem defined by (1)+BC with the initial condition $C_0=P_1(X,Y,Z,t)$. The procedure applied is the following:

a) The puff $P_1(X,Y,Z,t)$ is expressed as $P_1(X,Y,Z,t) = \sum_{l,m,n} C_{lmn}(t).H_{lmn}(X,Y,Z,0)$ using basis functions defined in the global coordinate system.

b) The basis functions $H_{lmn}(X,Y,Z,t)$ are re-defined in a frame with a rotated angle α calling it $H_{lmn}(x,y,z,t)$. α is related with the wind direction (see fig. 1). If the H_{lmn} is chosen appropriately, this step is trivial.

c) With the $C_{lmn}(t)$ found, $P_1(x,y,z,t+\Delta t)$ is calculated as

$$P_1(x,y,z,t+\Delta t) = \sum_{l,m,n} C_{lmn}(t).H_{lmn}(x,y,z,\Delta t)$$

d) The sought field $P_1(X,Y,Z,t+\Delta t)$ is defined afterwards as the image of $P_1(x,y,z,t+\Delta t)$ on the coordinate frame (X,Y,Z). This requires: 1) rotate the control points 2) calculate the grid values and 3) adjust the grid values so assure mass conservation in the transformation. Notice that the mass prior rotation is known, and the mass based on grid values varies linearly with them, so a correction coefficient can be calculated as

$$\frac{\sum C_{lmn}(t)\int_{\Omega} H_{lmn}(x,y,z,\Delta t)dxdydz}{\sum_{l,m,n}^{L,M,N} (grid\ values\ at\ t+\Delta t)\int_{\Omega} H_{lmn}(X,Y,Z,0)dXdYdZ}$$

and it can be applied straightforwardly to the grid values. L,M,N refers to the indexes of the grid values at $t+\Delta t$. It should be stressed that all the integrals in this equation can be calculated previously.

II) The case of the homogeneous initial condition with sources

Usually when there are point sources, they are irregularly distributed in the field. Due to the combined effects of the speed of discharge and buoyancy, the emission is not considered as taking place at the stack height, but higher up, at a virtual height identified as effective height h_e. In this case, source i is modeled following the function

$$S_i(X,Y,Z,t) = q_i(t).\delta(Z-h_e).\delta(X-X_i).\delta(Y-Y_i) \quad \textbf{(5)}$$

δ is Dirac's delta function and $q_i(t)$ is the strength of the i-th point source.

If the problem put forward in the equation (1) considers the i-th source alone, the boundary conditions, the initial condition $C_0(X,Y,Z,t)=0$ and takes (X_i,Y_i) as the origin, the following solution is obtained:

$$C(x,y,z,t+\Delta t) = q_i(t).Q_i(x,y,z,\Delta t) \quad \textbf{(6)}$$

Q $(x,y,z,\Delta t)$ is only related to the effective stack height.

Therefore, when dealing with the emission from a group of stacks, the following procedure is suggested (see fig. 2):

a) For each i, the effective height is calculated and then the pollutant field $Q_i(x,y,z,\Delta t)$ is found. The system of coordinates is rotated and displaced so as to express the field Q_i as $Q_i(X,Y,Z,t+\Delta t)$ in the "absolute" coordinate system. As before, $Q_i(x,y,z,\Delta t)$ is expressed as a Bezier surface, and mass adjusting is also required after rotation.

b) This same procedure is applied to all possible i, adding up all the values thus obtained.

$$Q(X,Y,Z,t+\Delta t) = \sum_{i}^{I} q_i(t).Q_i(X,Y,Z,\Delta t) \quad \textbf{(7)}$$

As mentioned above, in the following time step t+Δt, Q(X,Y,Z,t+Δt) will be considered as a summation of regular puffs.

In short: if the following field is considered, valid for t+Δt

$$C(x,y,z,t+\Delta t) = \sum_{l,m,n}^{L,M,N} C_{lmn}(t).H_{lmn}(x,y,z,\Delta t) + \sum_{i}^{I} q_i(t).Q_i(X,Y,Z,\Delta t)$$

By mere substitution it may be confirmed that it is a solution of (1)+BC with initial condition

$$C_0(x,y,z,t) = \sum_{l,m,n}^{L,M,N} C_{lmn}(t).H_{lmn}(x,y,z,0)$$

The ideas developed so far can be applied to the case of linear and area distributed sources, without additional problems.

3. ANALYSIS OF THE CHOSEN HYPOTHESES

a) *"..the windfield is liable to being assimilated locally almost unidirectional"*

Prior to this work, Cisa, Guarga, Briozzo et al, 1990, carried out a study of the windfield applied to Uruguay in view of wind energy purposes. The basic methodology used by them was the same as the one used by Endlich et al, 1982, with few variants. The Uruguay terrain is nearly flat (below 500 m ASL). Once analyzed the main components of the wind field (see fig. 3 as an example), it was clear that the abovementioned hypothesis is valid about 97% of the time. For further details of the calculation of the patterns and the weighting coefficients mentioned above, I refer back to Endlich et al, 1982, or Cisa et al, 1990.

b) *"..parameters* Λ, W_D, K_H, K_V, V_D *have values that are not a function of travel distance to the sources ... those parameters are only function of height z above ground..."*

Reynolds et al, 1973, expressed that there are no systematic measurements that enable the evaluation of the coefficients K_V and K_H. They have used a former formulation by Eschenroeder, in which $K_V=K_V(u, z/H)$.
Khairul Alam and Seinfeld, 1981, modeled the problem, assuming that K_H and K_V are constant in the workspace.
Bessemoulin et al, 1974, tried out different expressions of K_V, which could depend or not on the distance from the source.
Ragland and Dennis, 1975, used a family of functions, discriminating between the terrain height, involving also the Monin-Obukov length L. Consequently, $K_V=K_V(z, L)$.
Nieuwstadt, 1981, quoted a formulation with a fit using

$$K_V = \frac{0.4.u_*.z.(1 - z/H)^{1.5}}{1 + 4.7z/L} = K_V\left(z, \frac{z}{H}, \frac{z}{L}\right)$$

Several formulae mentioned presents a major shortcoming: that they depend on the system of units used. Therefore, they are not representations which are universally valid to solve the problem.
However, I have referred to them because, there are a good number of examples that fall within my hypothesis.

c) *"..It shall be assumed that* K_V, *w(z=0) and w(z=H) and* W_D *do not vary according to x, y in what follows...."*

This hypothesis does not seem extreme, since there exists uncertainty among the values of the parameters themselves.

Conclusions:

As far as I am concerned, the definition of puff is the portion of space within which our hypotheses of uniformity, unidirectionality and the state of steadiness, etc. are fulfilled. It will always be possible to subdivide the workspace into smaller zones easily.

SUMMARY:

A methodology that makes the application of the K-theory possible, lowering computer costs, has been put forth in this work. In it, the study of the transient phenomena of the advection of pollutants is undertaken, considering that comparable time computer-cost to the algebraic formulation characteristic of the Gaussian plume, could be achieved.

The essential idea intended to take advantage of the linearity of the advection-diffusion equation and at the same time, generate a catalogue of cases by means of calculations made on a powerful computer in a one-time operation. In real time, a solution through the linear combination of analyzed cases has been attempted. The method is based on two hypotheses: flat topography and instantly locally unidirectional windfield.

Were the case to apply to urban diffusion, where usually few meteorological stations are available. However, these hypotheses do not seem excessively restrictive. Were the case one of mesoscale diffusion, a wind pattern analysis should be done prior and its results carefully studied.

ACKNOWLEDGMENTS

This work was started on the occasion of an exchange program between Spain and Latin America, held in Valencia, Spain (Cátedra de Mecánica de Fluidos de la Universidad Politécnica de Valencia: Chair of Fluid Mechanics at the Polytechnic University of Valencia) sponsored by the Spanish Ministry of Culture. I also wish to express my sincere gratitude to Dr. Vicente Espert, José Cataldo, and Uri Groisman, for their kind participation in the preparation of this work, at different stages.

REFERENCES

Bessemoulin, P. et Benaire, M., 1974: "Contribution a l'etude de la diffusion des polluants gazeux dans l'atmosphere" Atmospheric Environment, 8, 261-279

Cisa, A., Guarga, R., Briozzo, C., López Vázquez, C. et al, 1990: "Convenio para el estudio del Potencial Eólico Nacional: Informe Final" (National Wind Energy Evaluation Program: Final Report. (In Spanish)). Facultad de Ingeniería, Instituto de Mecánica de los Fluidos e Ingeniería Ambiental, Montevideo, Uruguay.

Endlich, R. M., Ludwig, F. L., Bhumralkar, C. M., and Estoque, M. A. 1982: "A Diagnostic model for Estimating winds at potential sites for wind turbines", J. Appl. Meteorol., 21, 1441-1454.

Foley, J.; van Dam, A.; Feiner, S. and Hughes, J. F., 1990: "Computer Graphics: Principles and Practice" 2nd. ed. Addison-Wesley, pp. 521-522.

Kahirul Alam, M. and Seinfeld, J. H. 1981: "Solution of the steady state, three dimensional atmospheric diffusion equation for sulfur dioxide and sulfate dispersion from point sources", Atmospheric Environment, 15, 1221-1225

Ludwig, F. L., Gasiorek, L. S. and Ruff, R. E., 1977: "Simplification of a Gaussian puff model for real-time minicomputer use", Atmospheric Environment, 11, 431-436

Ludwig, F. L., 1985: "User's Guide for a model of airflow and diffusion in complex terrain (MADICT)": SRI Project 5047

Nieuwstadt, F. T. and Van Dop, H.(editors) "Atmospheric turbulence and air pollution modeling; A course held in The Hague, 21-25 September 1981" D. Reydel Publishing Co. pp 76-77

Ragland, K.W. and Dennis, K., 1975: "Point source atmospheric diffusion model with variable wind and diffusivity models" Atmospheric Environment, 9,175-181

Reynolds, S. D., Roth, R. M. and Seinfeld, J. H. 1973: "Mathematical modeling of photochemical air pollution - I", Atmospheric Environment, 7, 1033-1061

Sheih, C. M., 1978: "A Puff pollutant dispersion model with wind shear and dynamic plume rise", Atmospheric Environment, 12, 1933-1938.

Legend for figure 3:
Mass-consistent interpolation of the annual vector mean of the hourly windfield for 1990. Grid size is about 60Km