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A NEW GAUSSIAN PUFF ALGORITHM FOR NON-HOMOGENEOUS,
NON-STATIONARY DISPERSION IN COMPLEX TERRAIN

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ABSTRACT

This paper presents a complete algorithm for applying the Gaussian method to the most general and complex dispersion conditions. The plume evolution is described by transport and diffusion of a series of independent puffs, thus allowing the treatment of non-homogeneous, non-stationary conditions which characterize both short-range dispersion in complex terrain and long-range transport of pollutants. Physical and numerical problems related to the application of the puff model are discussed, and a general computer-oriented methodology proposed. This method provides a more numerically-accurate representation of plume characteristics and can handle both transport and calm conditions.

INTRODUCTION

Regulatory problems, especially in the U.S.A., have strongly affected air pollution dispersion studies. Recently, in fact, air quality modeling has been elevated in the U.S.A. to the quantitative decision-controlling level due, essentially, to the Clean Air Act Amendments of 1970 and 1977, and to the subsequent action of the U.S. EPA (U.S. EPA, 1978). Not only are mathematical models used for obtaining emission permits for existing sources, where field experiments allow some calibration and verification of the models, but due to a relatively new doctrine -- the Prevention of Significant Deterioration (PSD) -- air quality models are also one of the most important tools in industrial development and land use planning, especially in the Western United States.

Unfortunately, the accuracy of the applied modeling technique has not always been proportional to the importance of the regulatory problem. Oftentimes, with the justification that such methods provide "conservative" estimates, the physical assumptions used have been too simple for the simulation of very complex phenomena. More important, only recently has any attention been given to the problem of statistical evaluation of air quality model performance (Zannetti and Switzer, 1979; Hillyer et al., 1979; Bencala and Seinfeld, 1979).

Historically, the urgent need for simple, clear, and effective numerical methods for computing the environmental impact of an emission source has had the positive effect of boosting research and investigation in this field, but had the negative effect of forcing available methods to work beyond their physical and numerical limits.

A typical example is the extensive use of the Gaussian steady-state dispersion formula which has become -- and probably will remain for long time -- an essential regulatory tool for air pollution problems in the U.S.A. Such a methodology gives a plume formula whose validity requires the main assumptions of 1) spatial homogeneity, 2) stationary conditions, and 3) flat terrain. However, since many dispersion cases, especially in complex terrain or for intermediate ranges, do not follow these assumptions, much research has been and will be devoted to both the determination of empirical correction factors in the Gaussian approach and to the development of new algorithms for regulatory purposes.

In the past, the more complex, time-varying applications of air quality simulation modeling have made extensive use of dynamic grid model techniques (mainly finite-difference simulations following the K-theory approach). Recently, however, a growing concern has arisen regarding some important limitations of such a numerical approach and, precisely, of 1) its numerical advection errors, 2) its often incorrect representation of plume growth, and 3) the difficulty of relating the diffusion coefficient K to standard atmospheric measurements.

In addition, the whole Eulerian approach used in grid model simulations has been criticized, since a growing number of scientists agree in considering air pollution dispersion a Lagrangian phenomenon, to be simulated by specific source-receptor numerical methods, without the computation of spatially-averaged grid concentrations.

For the above reasons, some modelers have recently attempted to 1) develop new transport and diffusion techniques for the more complex applications (e.g., the particle-in-cell method; Sklarew et al., 1971; Lange, 1978), and 2) extend the applicability

of the Gaussian method by breaking up the plume into a series of independent elements, segments (Chan and Tombach, 1978), or puffs (Lamb, 1969) to treat, in particular, non-stationary, non-homogeneous dispersion conditions.

The following sections of this paper discuss the physical and numerical problems relating to the utilization of the puff method and define a new puff algorithm for both an accurate and computationally efficient simulation of plume characteristics by a series of puffs.

THE PUFF APPROACH

Puff Dispersion

In past dispersion studies (e.g., see Pasquill, 1974), puffs and plumes have shown different dispersion characteristics. In fact, while the spread of a plume (measured by the horizontal and vertical standard deviations of its spatial concentration distribution) tends initially to grow proportionally to the downwind distance and, ultimately, proportionally to the square root of such a distance, puff dispersion characteristics have shown different behaviors. In particular, Gifford (1957), in examining smoke puff data, found the existence of two predicted (Batchelor, 1952) growing regimes for the puff sigma, with an initial proportionality to the downwind distance, followed by a sigma growth proportional to the $3/2$ power of such a distance for intermediate dispersion.

Puff Modeling

In spite of the above considerations, most of the practical applications of puff modeling algorithms have avoided the treatment of real puff dispersion characteristics. In fact, it has been found that a Gaussian plume can be represented by a series of "equivalent" (or "fictitious") puffs if 1) the puff sigmas grow in the same way as the plume sigmas, and 2) the distance between two contiguous puffs is sufficiently small. Then, the existence in the computational domain of many puffs, instead of a stationary plume, allows some degree of representation of non-stationary, non-homogeneous emission and dispersion conditions, otherwise impossible to handle with standard Gaussian formulae.

However, this approach must not be seen as a perfect representation of the dispersion phenomenon. In particular, if the utilization of a plume sigma function for puff modeling is correct in nearly-stationary conditions, very little is known of its use during fully non-stationary situations and, especially, in nearly-calm conditions, which are often associated with air pollution episodes.

In conclusion, the common "puff model" must be considered only a step ahead in the application of the Gaussian semi-empirical approach. However, the method is potentially very powerful and future data on tracer dispersion experiments are expected to strongly improve the applicability of the entire methodology.

The Basic Puff Algorithm

The primary computational algorithm of the puff model consist of five computational substeps at each time step Δt .

1. Emission. One puff is generated at each emission exit point (plus, the eventual additional elevation due to the plume rise contribution).
2. Advection. The center of each existing puff is moved according to the local wind.
3. Diffusion. All puffs sigmas are increased according to the local turbulence state.
4. Deposition, Precipitation Scavenging, and Chemical Decay. The mass of each puff is reduced (e.g., by exponential reduction) to take these effects into account.
5. Contribution to Receptors. The contribution to each receptor is computed by summing all single contributions of the existing puffs.

Figure 1 shows an example of puff dispersion simulation (on a horizontal plane) from two point sources, where three-dimensional, non-stationary, non-homogeneous meteorological conditions can be properly taken into account by the method.

Recent improvements of the puff model have been developed for taking into account wind shear effect, dynamic plume rise (Sheih, 1978), and determining the correct time increment Δt for puff advection and diffusion computations (Ludwig et al., 1977). The latter problem is especially important to maintain an accurate plume representation without creating serious problems of computer storage and CPU running time, caused by a too small Δt . The solutions proposed for this problem consist of a puff-merging algorithm (Ludwig et al., 1977) and the incorporation of the mean-wind advection into the streamwise dispersion coefficient (Sheih, 1978). However, these methods are practical for use only in nearly steady-state conditions, since it can be easily proved that fully non-stationary simulations can require a computationally prohibitive Δt of a few seconds to avoid concentration overestimation and/or underestimation due to sudden changes of wind direction. In fact, the basic condition for a perfect representation of a Gaussian

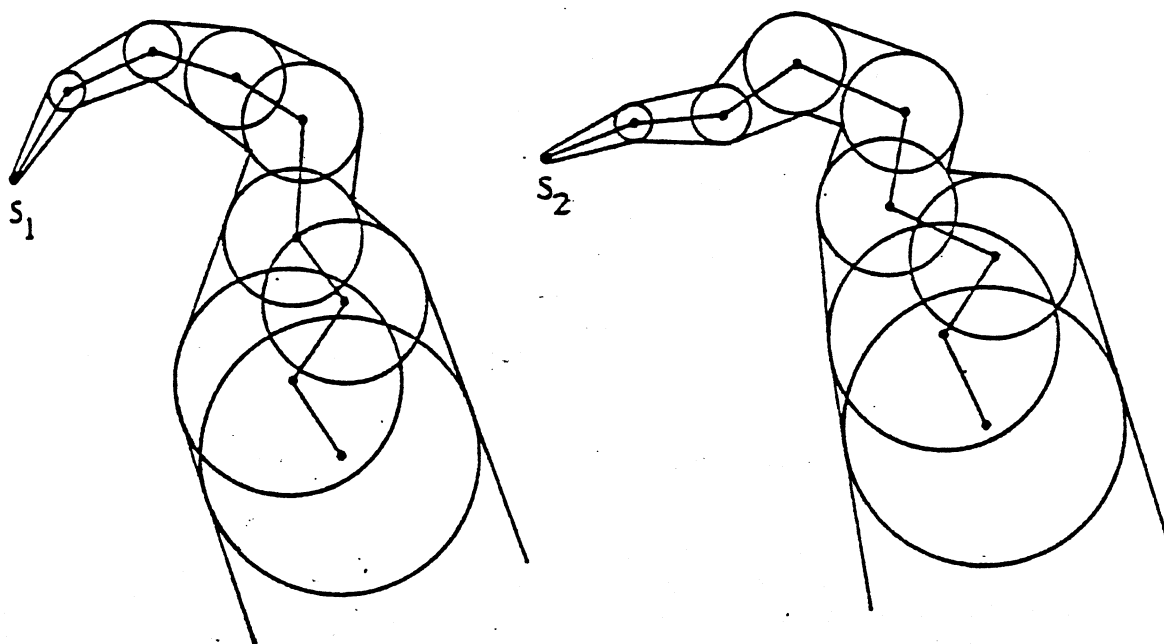


Fig. 1. Example of puff model dispersion computation (two point sources) in non-stationary, non-homogeneous meteorological conditions.

plume, by a series of independent puffs, requires the distance between the centers of two contiguous puffs to be less than their streamwise standard deviation of the concentration distribution (Ludwig et al., 1977); a condition that requires a too small Δt for concentration computations at receptors not too far from the source.

THE AVPPM^(*) METHOD

A new method has been proposed (Zannetti, in press) for a more accurate plume simulation by a series of puffs. This method handles general non-stationary conditions without creating serious computer storage and CPU time-consumption, as mentioned in the previous section. Moreover, a general algorithm has been incorporated for treating calm conditions.

The entire methodology has been codified into a computer package (AVPPM/2A) which, if a suitable meteorological input is available, seems particularly appropriate for the numerical simulation of non-homogeneous dispersion conditions (as in complex terrain) or non-stationary phenomena (as in intermediate or long-range dispersion simulations).

Representation and Handling of Puffs

The key point in the AVPPM algorithm is the selection of a Δt large enough (e.g., 5 to 10 minutes) to avoid serious computer storage and CPU time-consumption problems. However, such a large Δt provides a poor resolution for the plume description, since, the basic puff condition (separation between contiguous puffs less than their streamwise sigmas) is met only very far downwind of the source. In other words, the puffs give only the geometry of the plume's evolution and the puffs' masses cannot be used directly for computing the concentration at the receptor points.

Figure 2 shows a non-stationary plume represented by puffs at time intervals t and $t + \Delta t$. If a "chain" is kept between the puffs, their ages and source points at each time interval $[t, t + \Delta t]$, then the area affected by the entire plume (see Figure 2) can be represented by a certain number of quadrilaterals with vertices in the puffs' centers at the beginning and end of the time interval. Then, if a receptor is sufficiently close to a quadrilateral (e.g., less than 4 or 5 puffs' horizontal sigmas), a splitting technique is applied to generate enough puffs in the quadrilateral to meet the basic puff condition discussed above.

(*) AeroVironment Puff Plume Model

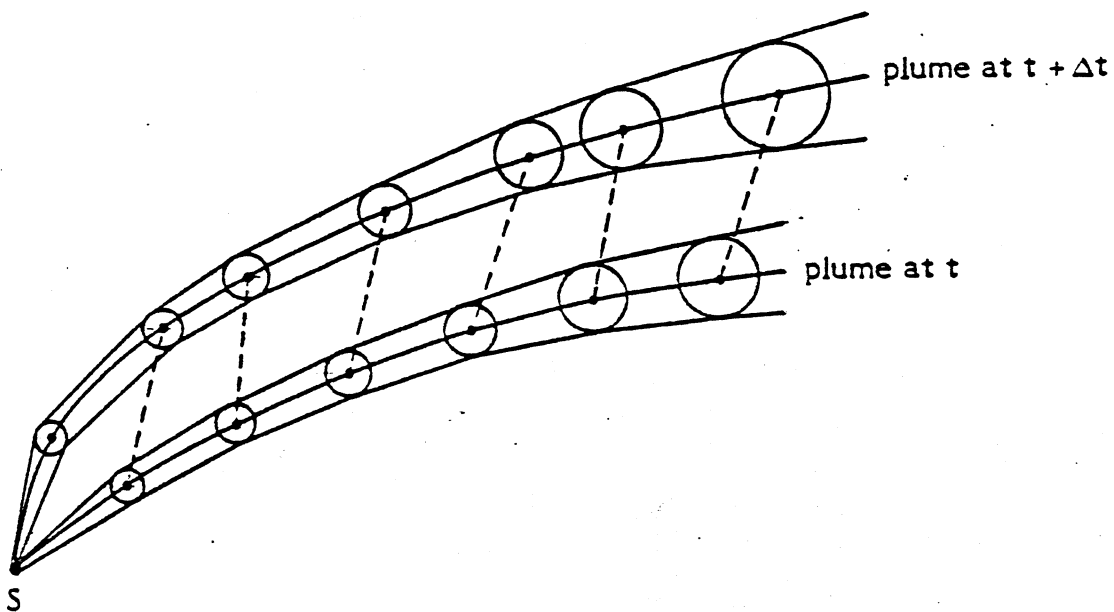


Fig. 2. Plume horizontal representation by a series of puffs at different time steps during non-stationary, non-homogeneous conditions. The mass of each puff; during the time interval $[t, t + \Delta t]$, has actually affected the area of the corresponding quadrilateral.

It must be noted that this splitting technique will be applied only when required for a particular receptor. In this way, we solve our computer storage and time problems without losing the accuracy of the computation.

Treatment of Calm Conditions

The AVPPM methodology assumes that, in the study area, wind speeds greater than u_{\min} define transport conditions, while wind speeds less than u_{\min} are associated with calm conditions, where u_{\min} must be determined from experimental data (a first guess can be 1 m/s).

We can then assume, in transport conditions, for example, the common power law:

$$\sigma = a d^b, \quad (1)$$

where the sigma evolution of each puff is a function of the downwind distance d , and the parameters a and b are dependent upon the turbulence state.

In calm conditions, statistical considerations of the turbulence characteristics (Pasquill, 1974) allow the description of a similar sigma growing law

$$\sigma = a' (t - t_0)^{b'}, \quad (2)$$

where $t - t_0$ is the age of the puff since its generation at t_0 .

Then, for wind speed u equal to u_{\min} , Equations (1) and (2), using $d = u (t - t_0)$, give

$$a' = a u_{\min}^b, \quad b' = b. \quad (3)$$

The AVPPM algorithm in the puff diffusion step uses Equation (1) for transport conditions and Equation (2) for calm conditions, where a' and b' are given by Equation (3).

The above methodology is not restricted to the sigma function of Equation (1), since similar considerations can be developed for virtually any sigma function. However, the above scheme should provide a first approximation algorithm for a consistent treatment of calm conditions, where future tracer experiments are expected, in particular, to supply a better estimation of a' and b' .

Virtual Distances and Ages

At each time step, diffusion is taken into account by increasing the sigmas of each puff. In transport conditions, for example, from Equation (1) we have

$$\Delta\sigma = \frac{\partial\sigma}{\partial d} \Delta d = abd^{b-1} \Delta d, \quad (4)$$

where Δd is the distance traveled by the puff during Δt .

The dependence of $\Delta\sigma$ on the total downwind traveling distance d requires particular care and special consideration. It is easy to see, in fact, that the real downwind distance d is not generally appropriate for this computation. Figure 3 shows the time evolution of a single puff where a change in the turbulence state at time t (in our case, an increase of turbulence) changes the growing rate of the puff's sigmas. It is clear that, after time t , the puff growth is affected not by the total actual downwind distance d , but by the "virtual" downwind distance d_v from the virtual source S' . This virtual distance d_v is defined as the downwind distance that the same puff, to have the same sigmas, would have had to travel from the source if the turbulence state had always been the most recent one during its entire life.

More generally, with different horizontal and vertical turbulence characterizations, virtual distances of a horizontal d_h and vertical d_v , should be defined. Moreover, when the puff grows according to its age (in calm conditions), similar considerations are brought to the definition of a virtual age t_v or, more generally, of a horizontal t_h and vertical t_v virtual ages of the puff.

According to the above considerations, the increase of the puff's sigmas at time t , assuming Equations (1) and (2), is computed using

$$d_v = [\sigma(t)/a^*]^{1/b^*}, \quad (5)$$

and

$$t_v = [\sigma(t)/a'^*]^{1/b'^*}, \quad (6)$$

where a^* and b^* are the coefficients of Equation (1) for the current turbulent state j^* (at time t) computed at the puff's center, and a'^* , b'^* are the analogous coefficients of Equation (2).

As a final important remark on this method, it must be pointed out that the sigma power law of Equation (1) is not essential for the algorithm. Any general formula

$$\sigma = f[d] \quad (7)$$

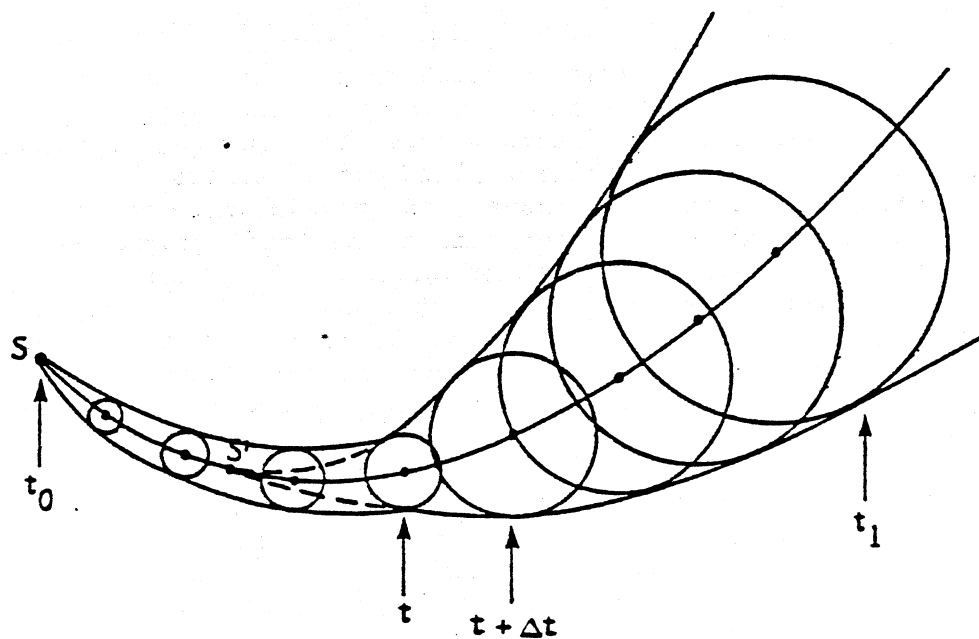


Fig. 3. Evolution of one puff during the time interval $[t_0, t_1]$. Turbulence is low during $[t_0, t]$ and increases during $[t, t_1]$, then requiring the computation of the virtual distance of the puff from the virtual source S' .

can be used, then requiring

$$d_v = f^{-1}[\sigma(t)], \quad (8)$$

for the computation of the virtual distance.

However, with formulae more complex than Equation (1), the computation of Equation (8) is not straightforward as in Equation (5) and, consequently, an iterative algorithm may be required. Analogous considerations hold for the virtual age.

CONCLUSIONS

A new puff dispersion algorithm for plume representation has been discussed. The utilization of this methodology should increase the applicability of the Gaussian method to treat both non-stationary, non-homogeneous conditions, and calm conditions.

The puff method discussed above has been codified into a computer package (AVPPM/2A) which, with suitable input data on wind, turbulence, and emissions, can simulate dispersion experiments using various options on sigma parameters, plume rise functions, ground and inversion reflection parameters, etc. Moreover, for complex terrain simulations, the elevation above the ground of the center of each puff is forced, from one step to the next, to remain within a pre-fixed range to better take into account terrain irregularities.

The code has been successfully compared against steady-state Gaussian computations. As an example, simulations that required Δt of the order of 10 seconds, according to the basic puff condition, have been correctly performed with a Δt of one order of magnitude greater.

However, simulation runs have pointed out the importance of using an accurate splitting technique. In fact, in some cases, the generation of artificial puffs, by a linear interpolation of the characteristics of the four puffs at the vertices of the quadrilateral, does not provide sufficient accuracy.

Numerical tests using a correct interpolation technique have shown that a more accurate computation is particularly important for splitting inside the first quadrilateral (the one which contains the source), where the highest error is produced by simple linear interpolation. However, if some attention is paid to the choice of Δt , the computationally faster linear interpolation can be successfully used.

Experimental data are expected soon which will validate the entire methodology, especially the semi-empirical method which has

been proposed for the treatment of calm conditions. Data are also expected to suggest concentration distributions different from the Gaussian one and easily incorporable into the method.

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