ENVIROSOFT 86

Proceedings of the International Conference on Development and Application of Computer Techniques to Environmental Studies, Los Angeles, U.S.A., November 1986

Editor:
P. Zannetti

A Computational Mechanics Publication

A Non-Gaussian Climatological Model for Air Quality Simulations

T. Tirabassi, M. Tagliazucca
FISBAT-CNR, via de' Castagnoli, I-40126 Bologna, Italy
P. Zannetti
AeroVironment Inc., 825 Myrtle Avenue, Monrovia, California 91016, U.S.A.

ABSTRACT

A non-Gaussian climatological model for air quality dispersion simulations is presented. The model uses a two-dimensional analytic solution of the advection-diffusion equation. The solution is obtained using power-law functions of height for the wind speed and the vertical exchange coefficient. The climatological version of this formula provides a methodology for computing long-term average concentrations (e.g., annual averages) generated by emission sources. The model is implemented in FORTRAN language and can run in virtually any computer. A flow chart of the main program is presented.

INTRODUCTION

Theoretical analyses of the diffusion of material in a turbulent flow have developed along three main lines: (i) the gradient transfer approach; (ii) the statistical theory of turbulent velocity fluctuations; and, (iii) similarity considerations. In this third line of development, the laws relating the diffusion coefficients to the controlling physical parameters are derived on a dimensional basis. The statistical theory is essentially a kinematic approach in which the behavior of marked elements of turbulent fluid is described in terms of given statistical properties of the motion. The gradient-transfer approach assumes that turbulence causes a net movement of pollutants in the opposite direction to the gradient of pollutant concentration, at a rate proportional to the magnitude of the gradient. The proportional factor is analogous to the coefficient of viscosity or conductivity in the familiar laws for the transfer of momentum or heat in laminar flow.

The differential equation that has been the starting point of most mathematical treatments of atmospheric diffusion is a generalization of the classical equation for heat conduction in a solid, and is essentially a statement of the conservation of the suspended material.

The history of the analytic solutions of the advection-diffusion equation of air pollutants began in the mid 1800's, when Albert Fick, a German physiologist, was able to describe the special case of dispersion with a diffusion coefficient independent of position.

Roberts[1] gave the first solution of the diffusion equation, in both a vertically isotropic and a vertically anisotropic atmosphere. However, his solution is valid only for a ground-level source, given vertical profiles of the wind speed and the eddy exchange coefficient expressed by power laws. In the following years, much more attention was paid to the isotropic solution and to the empirical determination of the lateral and vertical standard deviations of the concentration distribution to correctly fit the experimental data (Pasquill[2]). Up to now, an enormous amount of work has been done to support and improve the so-called Gaussian approach. The anisotropic solution, on the other hand, got on slowly. In fact, only in 1975, Yeh and Huang[3] and Berlyand[4] found a two-dimensional solution, valid also for an elevated source, for an infinite boundary layer characterized by power law profiles of the wind velocity and of the vertical eddy exchange coefficient. In 1978, Demuth[5] extended the solution to a limited boundary layer and, in 1979, Huang[6] suggested setting up a three-dimensional solution by describing horizontal diffusion with a Gaussian term. Currently, analytic solutions cannot incorporate general profiles of the wind speed and the vertical eddy exchange coefficient. Such situations can be described more accurately by numerical solutions, but these require complicated and time-consuming computer routines.

General analytical solutions of the advection-diffusion equation use simpler formulas that have been incorporated into several computer packages. For the computation of long-term average concentrations, climatological models are available. They are based on the Gaussian solution, which simulates atmospheric diffusion using semi-empirical sigma functions, in spite of the theoretical deficiencies due to the vertically anisotropic characteristics of the atmospheric turbulence.

Our purpose in this paper is to fill the gap by suggesting a new computer routine for climatological models based on a non-Gaussian analytic solution (Yeh and Huang[3], Berlyand[4], Demuth[5]) for power-law vertical profiles of the wind speed and the eddy exchange coefficients.

Here we present the climatological form of a three-dimensional model (KAPPA-G) set up with the above analytical solutions to compute vertical diffusion, while horizontal diffusion is simulated by the Gaussian formula. This three-dimensional model has been implemented in a computer package (KAPPA-G) written in standard FORTRAN language. Its performance has been evaluated by comparison with data from SF6 tracer experiments (Tagliazucca et al.[7] and Tirabassi et al.[8]).

THE ANALYTIC SOLUTION

The steady-state, advection-diffusion equation that describes the dispersion of a passive material released by an elevated point source, advected by an x-directed mean wind profile u(z) and diffused by the action of turbulent exchange coefficients $K_x(z)$, $K_y(z)$ and $K_z(z)$, is approximately

$$u \frac{\partial}{\partial x} C = \frac{\partial}{\partial z} (K_z \frac{\partial}{\partial z} C) + \frac{\partial}{\partial y} (K_y \frac{\partial}{\partial y} C) \tag{1}$$

if

$$\left| u \frac{\partial}{\partial x} C \right| >> \left| \frac{\partial}{\partial x} \left(K_x \frac{\partial}{\partial x} C \right) \right| .$$

The source condition is

$$C = \frac{Q}{u(H_e)} \delta(z - H_e)\delta(y) \quad \text{as } x \to 0$$

where C=C(x,y,z) is the mean concentration field, Q is the emission intensity of the source placed at (0, 0, H_e), H_e is the effective height of the source (H_e = H_e + DH), and DH is the plume rise. δ means the delta function.

The boundary conditions are:

$$K_z \frac{\partial C}{\partial z} = 0 \quad \text{at } z = 0,H$$

where H is the height of the mixing layer. Moreover,

$$u(z) = u_0(z/h_0)^\alpha$$

$$K_z = K_z(z) = K_{z0}(z/h_0)^\beta$$

$$K_y = u(z)f(x)$$

where h_0 is the height where u_0 and K_{z0} are evaluated and f(x) is a function of x.

The solutions of equation (1) are presented in Table 1, while Table 2 shows the same solutions for ground-level concentrations.

$$C(x,y,z) = \overline{C}(x,z)\,\frac{1}{\sqrt{2\pi}\,\sigma_y}\exp\left(-\frac{y^2}{2\sigma_y^{\,2}}\right)$$

Unbounded atmosphere ($H = +\infty$)

$$\overline{C}(x,z) = \frac{Q(zH_e)^p h_0^{\beta}}{\lambda K_{z0} x}\exp\left(-\frac{u_0 h_0^{r}(z^{\lambda} + H_e^{\lambda})}{\lambda^2 K_{z0} x}\right) \times I_{-\nu}\left(\frac{2u_0 h_0^{r}(zH_e)^q}{\lambda^2 K_{z0} x}\right)$$

Bounded atmosphere ($H < +\infty$)

$$\overline{C}(x,z) = \frac{2Qqh_0^{\alpha}}{H^{\alpha+1}u_0}\left\{\lambda + \left(\frac{zR}{H}\right)^p \times \sum_{i=1}^{\infty}\left[\frac{J_{\gamma-1}(\sigma_{\gamma(i)}R^q)J_{\gamma-1}[\sigma_{\gamma(i)}(z/H)^q]}{J_{\gamma-1}^{\;2}(\sigma_{\gamma(i)})} \times \exp\left(-\frac{\sigma_{\gamma(i)}^{\;2}q^2K_{z0}x}{H^{\lambda}h_0^{r}u_0}\right)\right]\right\}$$

Conditions

$u(z) = u_0(z/h_0)^{\alpha}$ $\qquad K_y = u(z)f(x)$ $\qquad K_z = K_z(z) = K_{z0}(z/h_0)^{\beta}$

Table 1: Analytic solution equations. C is the pollution concentration, x is the along-wind direction, z is the height, Q the source emission, σ_y the lateral standard deviation, H_e the source effective height, u the wind velocity, K_z and K_y the vertical and lateral eddy exchange coefficients, h_0 the height where u_0 and K_{z0} are evaluated, H the mixing height, $\lambda=\alpha-\beta+2$, $\nu = (1-\beta)/\lambda$, $\gamma = (\alpha+1)/\lambda$, $r = \beta-\alpha$, $R = H_e/H$, $p = (1-\beta)/2$, $q = \lambda/2$, I_ν and J_ν represent the Bessel function and modified Bessel function of first kind and order ν, $\sigma_{\gamma(i)}$ the roots of J_ν and f(x) any function of x.

Unbounded atmosphere (H = + ∞)

$$\bar{C}(x,0) = \frac{Q}{\lambda^{\eta}} \frac{1}{\Gamma(\gamma)} \frac{h_0^{\eta}}{u_0^{\nu}\,(xK_{z0})^{\gamma}} \exp\left[- \frac{u_0 h_0^{r} H_e^{\lambda}}{\lambda^2 K_{z0} x} \right]$$

Bounded atmosphere (H < + ∞)

$$\bar{C}(x,0) = \frac{2Qqh_0^{\alpha}}{H^{\alpha+1}u_0} \left\{ \gamma + R^p \sum_{i=1}^{\infty} \left[\frac{J_{\gamma-1}(\sigma_{\gamma(i)}R^q)\sigma_{\gamma(i)}^{\gamma-1}}{\Gamma(\gamma) J_{\gamma-1}^{2}(\sigma_{\gamma(i)}) 2^{\gamma-1}} \times \exp\left(- \frac{\sigma_{\gamma(i)}^{2} q^2 K_{z0} x}{H^{\lambda} h_0^{r} u_0} \right) \right] \right\}$$

Table 2: Analytic solution equations for ground level concentrations. The symbols are the same as in Table 1 but $\eta = (\alpha+\beta)/\lambda$ and Γ denotes the Gamma function.

THE CLIMATOLOGICAL MODEL

The climatological model uses the same basic assumptions as the short-term KAPPA-G model (Tirabassi et al.[8]). As a peculiarity of the climatological model, however, the area surrounding the continuous source of pollutants is divided into sectors of equal angular width. The program requires, as meteorological input, the seasonal or annual frequency distribution of wind direction, computed in the same angular sectors.

Seasonal or annual emissions from the source are attributed to each sector according to the frequencies of wind blowing toward that sector. The ground-level concentration fields calculated for each source are translated to a common coordinate system and added together to obtain the total due to all sources.

In mathematical notation, for a single stack located in the origin, the long-term average concentration at a point (r, θ), in polar coordinates, is given by:

$$C(r,\theta) = \frac{2\ 10^6}{\sqrt{2\pi}\ r\ \Delta\theta} \sum_{i,k} \frac{Q_{i,k}\ f_{i,k}(\theta)\ S_{i,k}}{\bar{u}_{e_{i,k}}} \cdot \exp\left[D_i \frac{r}{\bar{u}_{e_{i,k}}}\right]$$

where:

$C(r, \theta)$ is the ground level concentration at the point (r, θ) ($\mu g/m^3$)

$\Delta \theta$ is the sector width in radians.

$Q_{i,k}$ is the pollutant emission rate for the i^{th} stability category and k^{th} wind speed category (g/s); a different buoyancy is also associated to each $Q_{i,k}$.

$f_{i,k}$ is the relative frequency of occurence of the i^{th} stability category and k^{th} wind speed category for each direction θ.

$S_{i,k}$ is the vertical diffusion term for the i^{th} stability category and k^{th} wind speed category.

$\bar{u}_e$ is the wind speed at the effective plume height for the i^{th} stability category and k^{th} wind speed category (m/s).

D_i is the decay term due to the ground deposition and chemical transformations (s^{-1}) for the i^{th} stability category.

The model uses, in the term $S_{i,k}$, the solutions of Table 2. Moreover, it uses Briggs' formulation (Briggs[9]) for computing the plume rise. The vertical atmospheric stability is evaluated either by the Pasquill-Gifford stability classes or by the Monin-Obukhov length. The exponent α of the wind profile is evaluated by interpolating Irwin's[10] data, given the atmospheric stability and the terrain roughness, while the exponent β of the eddy exchange coefficient profile is obtained from Draxler's[11] data. Depletion of material due either to ground deposition or to chemical reactions is accounted for by the decay exponential term.

THE PACKAGE

The model is written in standard FORTRAN language and can run on virtually any computer. The receptor points are given by the user or automatically generated on either a rectangular or a polar grid of receptors.

Values of α and β for each stability class, for a given roughness, can be specified by users or, alternately, default values can be used (the α parameters proposed by Irwin[10] and the β parameters from Draxler[11])

Other default values are:

- wind speed classes are 9, as in standard Weather Bureau use;
- the sector width is $2\pi/16$ radians;
- the decay term D is equal to 0.

The flow chart of the main program is depicted in Figure 1.

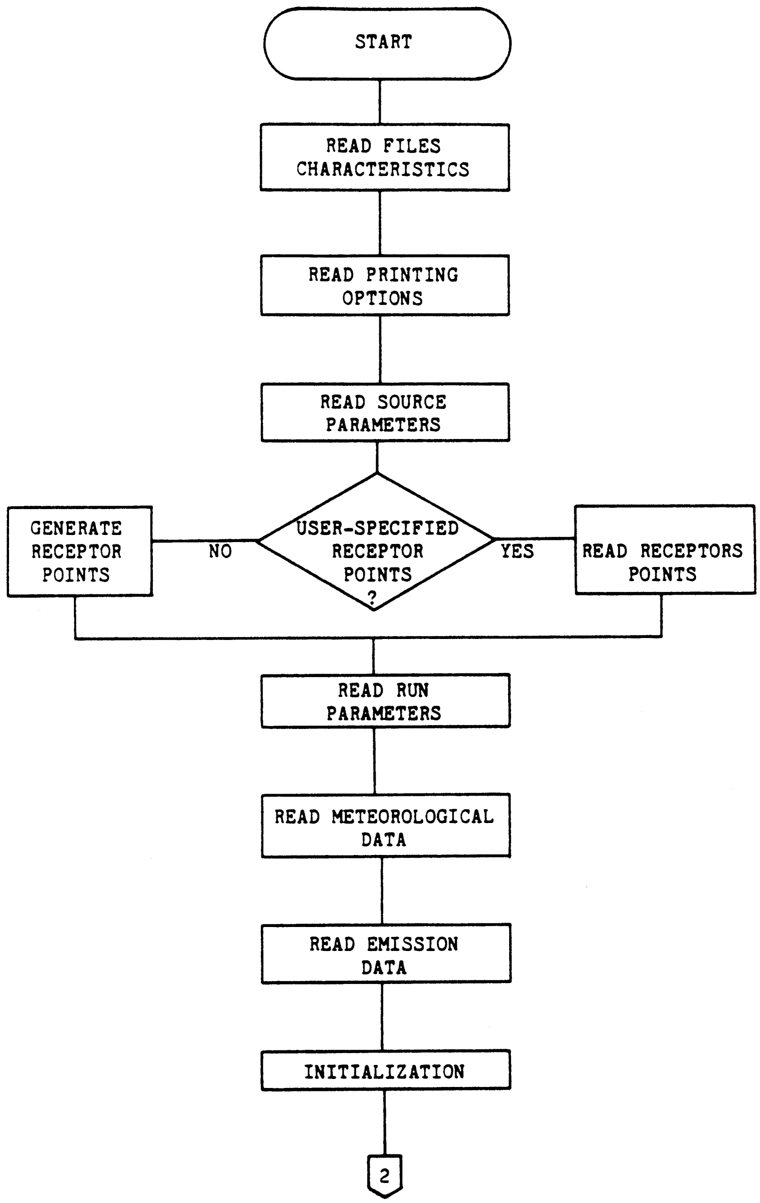

Figure 1. Flow Chart of the Main Program

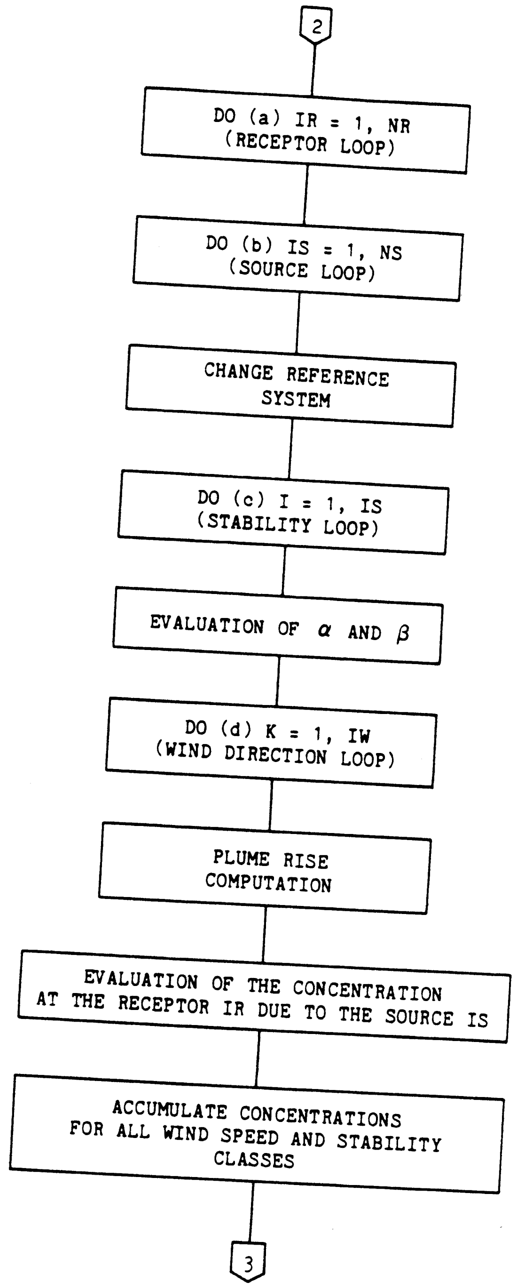

Figure 1. Flow Chart of the Main Program (Continued)

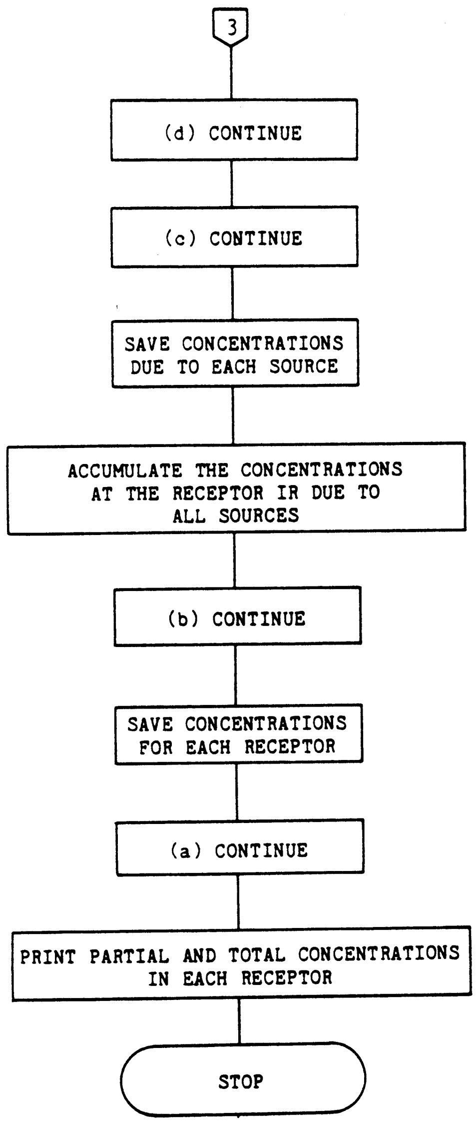

Figure 1. Flow Chart of the Main Program (Continued)

CONCLUSIONS

A non-Gaussian climatological model has been described. It uses a two-dimensional solution of the advection-diffusion equation, which has been analytically integrated using power law functions for the vertical profiles of the wind speed and the eddy exchange coefficient.

The climatological model is derived from a three-dimentional short-term model (KAPPA-G) that has been successfully validated for both sources in the surface layer (Prairie-Grass experiment data set; Tagliazucca et al.[7]) and tall stack emissions (EPRI-Kincaid data set; Tirabassi et al.[12], Tirabassi et al.[8]).

In order to avoid too much complexity with respect to the usual Gaussian climatological models, the vertical atmospheric inhomogeneities have been restricted to six classes of α and β, for each roughness length, which correspond to the usual six atmospheric stability classes.

The model will be improved in the future by computing α and β directly from vertical profile measurements instead of from stability classification. This approach will increase the complexity, but should provide a further improvement of the simulation capabilities of our climatological approach.

REFERENCES

1. Roberts, O.F.T (1923), The Theoretical Scattering of Smoke in a Turbulent Atmosphere, Proc. Roy. Soc., Vol. 104, pp. 640-654.

2. Pasquill, F. (1961), The Estimation of the Dispersion of Windborne Material, Met. Mag., Vol 90, pp. 33-49.

3. Yeh, G.T. and Huang, C.H. (1975), Three-Dimensional Air Pollutant Modelling in the Lower Atmosphere, Boundary Layer Meteor., Vol. 9, pp. 381-390.

4. Berlyand, M.Y. (1975), Modern Problems of Atmospheric Diffusion and Air Pollution, Translated Version by NEPC, USEPA, Raleigh, NC.

5. Demuth, C. (1978), A Contribution to the Analytical Steady Solution of the Diffusion Equation for Line Sources, Atmos. Environ., Vol. 12, pp. 1255-1258.

6. Huang, C.H. (1979), A Theory of Dispersion in Turbulent Shear Flow, Atmos. Environ., Vol. 13, pp. 453-463.

7. Tagliazucca, M., Nanni, T. and Tirabassi, T. (1975), An Analytical Dispersion Model for Sources in the Surface Layer, Nuovo Cimento, Vol. 8, pp. 771-781.

8. Tirabassi, T., Tagliazucca, M. and Zannetti, P. (1986), KAPPA-G, a Non-Gaussian Plume Dispersion Model: Description and Evaluation Against Tracer Measurements, JAPCA, Vol. 36, pp. 592-596.

9. Briggs, G.S. (1975), Plume Rise Prediction, Lectures on Air Pollution and Environmental Impact Analysis, pp. 59-111, American Meteorological Society, Boston.

10. Irwin, J.S. (1979), A Theoretical Variation of the Wind Profile Power Law Exponent as a Function of Surface Roughness and Stability. Atmos. Environ., Vol. 13, pp. 191-196.

11. Draxler, R.R. (1979), Estimating Vertical Diffusion from Routine Meteorological Tower Measurements, Atmos. Environ., Vol. 13, pp. 1559-1564.

12. Tirabassi, T., Tagliazucca, M. and Zannetti, P. (1985), Evaluation of a Dispersion Model Based on a Non-Gaussian Analytical Solution in Turbulent Shear Flow, Proceedings of DOE/AMS Model Evaluation Workshop, Chapter 4-2, Kiawah Island, U.S.A.