JAPCA 36: 592–596 (1986)

Reprinted from APCA Journal, Vol. 36, No. 5, May 1986

KAPPA-G, A Non-Gaussian Plume Dispersion Model: Description and Evaluation Against Tracer Measurements

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This paper presents a mixed methodology for the simulation of atmospheric disperson phenomena in which vertical diffusion is computed using an analytical solution of the *K*-theory equation, while horizontal diffusion is simulated by the Gaussian formula. This new formulation, while maintaining a simple analytical form for the concentration field, incorporates the effects of power-law vertical profiles of both wind speed and eddy diffusivity. The performance of this approach, which has been implemented into a full computer package (KAPPA-G), is evaluated by comparison with data from SF_6 tracer experiments.

Transport and diffusion models of air pollution are based either on simple techniques, such as the Gaussian steady-state analytical equation, or on more complex algorithms, such as the K-theory differential equation. The Gaussian equation is an easy and fast method which, however, cannot properly simulate complex nonhomogeneous conditions in a three-dimensional domain. The K-theory can accept virtually any complex three-dimensional meteorological input, but generally requires a finite-difference numerical integration which is computationally expensive and is often affected by large numerical advection errors.

However, the K-theory equation can be analytically solved in two dimensions under the following simplifying assumptions[1,2]:

1. Dispersion occurs in steady-state transport conditions.
2. The horizontal wind, u, is expressed as a power law function of height.
3. The vertical eddy diffusion coefficient, K_z, is expressed as a power law function of height.

Analytical solutions have been provided by several authors. Roberts (see Calder[3]) obtained a two-dimensional solution for ground level sources. Smith[4] found a solution for elevated sources with u and K_z profiles following Schmidt's conjugate law. Rounds[5] proposed a more general solution which, however, turned out to be valid only for linear profiles of K_z. Finally, Yeh and Huang[1] and Demuth[2] obtained a more general analytical solution which constitutes the numerical basis of our modeling approach for this study. We have implemented this methodology into an organized computer package, KAPPA-G, which allows the performance of three-dimensional steady-state simulations using the Gaussian formula for the treatment of horizontal diffusion (as proposed by Huang[6]). In many applications, this approach is preferable to the steady-state Gaussian three-dimensional equation, because it better represents the vertical stratification of the atmosphere, and especially, the wind shear. The main objective of this paper is, therefore, to illustrate the KAPPA-G method and its advantages with respect to standard Gaussian modeling formulations.

The next section presents a detailed analytical description of the proposed modeling approach, together with its parameterizations and assumptions. This is followed by a preliminary performance evaluation of the model, obtained by comparing model outputs with data collected during some of the SF_6 tracer experiments conducted by the Electric Power Research Institute (EPRI) at Kincaid, Illinois. The last section presents our conclusions and recommendations, and possible future developments.

The KAPPA-G Package

The computer package KAPPA-G is written in standard FORTRAN language and can run in virtually any computer. This package performs steady-state simulations of atmospheric diffusion phenomena under the assumptions and parameterizations described below.

The Analytical Solution of the *K*-Theory Equation

The steady-state advection and diffusion equation describing the dispersion of a passive material released by an elevated point source, transported by a mean wind profile $u(z)$ along x, and diffused by the action of turbulent eddy coefficients K_x, K_y, K_z can be approximately written:

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

with initial condition

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

and boundary conditions

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

where $C(x,y,z)$ is the mean concentration field of the passive material, Q is the emission rate of the release at $(0,0,H_e)$, H_e is the final effective height of the emission source, H is the depth of the mixing layer, δ is the delta function, and

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

We assume dispersion occurs in flat terrain with the following assumptions

$$u(z) = u_0(z/h_0)^{\alpha} \tag{2a}$$

$$K_z = K_z(z) = K_{z0}(z/h_0)^\beta \tag{2b}$$

$$K_y = u(z)f(x) \tag{2c}$$

$$H = +\infty \tag{2d}$$

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

Consider the crosswind integrated concentration

$$\overline{C}(x,z) = \int_{-\infty}^{+\infty} C(x,y,z)dy.$$

Then the solution[1] of Equation 1 for ground level concentration ($z = 0$) is

$$\overline{C}(x,0) = \frac{Q}{\lambda^\eta}\frac{1}{\Gamma(\gamma)}\frac{h_0^\eta}{u_0^\nu\,(xK_{z0})^\gamma}\exp\left[-\frac{u_0 h_0^r H_e^\lambda}{\lambda^2 K_{z0}x}\right] \tag{3a}$$

where $\lambda = \alpha - \beta + 2$

$\nu = (1 - \beta)/\lambda$

$\gamma = (\alpha + 1)/\lambda$

$\eta = (\alpha + \beta)/\lambda$

$r = \beta - \alpha$

and Γ denotes the Gamma function.

With a finite mixing height ($H < +\infty$) and $H_e < H$ (with the other assumptions in Equations 2a–2d unchanged), the solution[2] of Equation 1 is

$$\overline{C}(x,0) = \frac{2Qqh_0^\alpha}{H^{\alpha+1}u_0}\left\{\gamma + R^p\sum_{i=1}^{\infty}\left[\frac{J_{\gamma-1}(\sigma_{\gamma(i)}R^q)\sigma_{\gamma(i)}{}^{\gamma-1}}{\Gamma(\gamma)J_{\gamma-1}{}^2(\sigma_{\gamma(i)})2^{\gamma-1}} \times \exp\left(-\frac{\sigma_{\gamma(i)}{}^2q^2K_{z0}x}{H^\lambda h_0^r u_0}\right)\right]\right\} \tag{4a}$$

where $R = H_e/H$

$p = (1 - \beta)/2$

$q = \lambda/2$

$J_\gamma(\ldots)$ represents the Bessel function of the first kind and order γ; and $\sigma_{\gamma(i)}$, ($i = 1,2,\ldots$) are its roots, i.e., $J_\gamma(\sigma_{\gamma(i)}) = 0$.

The solutions given by Equations 3a and 4a both represent the case when $z = 0$. If elevated integrated concentrations $\overline{C}(x,z)$ need to be evaluated, the new solution, for $H = +\infty$, is easily obtained from Huang,[6] giving

$$\overline{C}(x,z) = \frac{Q(zH_e)^p h_0^\beta}{\lambda K_{z0}x}\exp\left(-\frac{u_0h_0^r(z^\lambda + H_e^\lambda)}{\lambda^2K_{z0}x}\right) \times I_{-\nu}\left(\frac{2u_0h_0^r(zH_e)^q}{\lambda^2K_{z0}x}\right) \tag{3b}$$

where $I_{-\nu}(\ldots)$ is the modified Bessel function of the first kind and order $-\nu$.

If $H < +\infty$, the integrated concentration $\overline{C}(x,z)$ is again obtained from Demuth,[2] giving

$$\overline{C}(x,z) = \frac{2Qqh_0^\alpha}{H^{\alpha+1}u_0}\left\{\lambda + \left(\frac{zR}{H}\right)^p \times \sum_{i=1}^{\infty}\left[\frac{J_{\gamma-1}(\sigma_{\gamma(i)}R^q)J_{\gamma-1}[\sigma_{\gamma(i)}(z/H)^q]}{J_{\gamma-1}{}^2(\sigma_{\gamma(i)})} \times \exp\left(-\frac{\sigma_{\gamma(i)}{}^2q^2K_{z0}x}{H^\lambda h_0^r u_0}\right)\right]\right\} \tag{4b}$$

We verified, analytically or numerically, that as $z \to 0$, the limit of Equations 3b and 4b gives Equations 3a and 4a, respectively; and that, as $H \to +\infty$, the limit of Equations 4a and 4b gives Equations 3a and 3b, respectively.

The above formulas dealt with the cross-wind integrated concentration $\overline{C}(x,z)$. If we assume that the plume has a Gaussian concentration distribution in the horizontal with lateral standard deviation $\sigma_y(x)$, we obtain

$$C(x,y,z) = \overline{C}(x,z)\frac{1}{\sqrt{2\pi}\sigma_y}\exp\left(-\frac{y^2}{2\sigma_y{}^2}\right). \tag{5}$$

Equation 5 can be correctly used for three-dimensional simulations, since the Gaussian assumption for horizontal diffusion gives

$$K_y = \frac{u}{2}\frac{d\sigma_y{}^2}{dx}$$

which always satisfies the condition of Equation 2c. Equation 5 has been selected as the basic numerical algorithm for our dispersion algorithms.

The Plume Rise

KAPPA-G utilizes the Briggs[7] formulation for computing the dynamic plume rise $\Delta h(x)$. Therefore, the effective height H_e is a function also of the downwind distance x.

Model's Input

KAPPA-G is very flexible in the definition of the meteorological input. The minimum information required, besides emission characteristics, is

1. The wind speed measured at some height.
2. The vertical atmospheric stability [either a Pasquill-Gifford (PG) stability class or the Monin-Obukhov length L].
3. The horizontal atmospheric stability (either a PG stability or the standard deviation of the horizontal wind direction σ_θ).

The package can extrapolate this minimum information to compute full vertical profiles. However, if vertical meteorological profiles are available, they can be used directly by the package.

In particular, the exponent α of the power law profile of u is computed by fitting a power law to the measured wind profile. This process requires the two profiles to coincide at the final effective source height H_e and to have the same average advective flux between the ground and H_e. That is,

$$u_p(H_e) = u_a(H_e) \tag{6a}$$

$$\frac{1}{H_e}\int_0^{H_e} u_p(z)dz = \frac{1}{H_e}\int_0^{H_e} u_a(z)dz = \bar{u} \tag{6b}$$

where u_p is the power law fitting and u_a is the actual measured profile. It follows that

$$\alpha = [u_p(H_e) - \bar{u}]/\bar{u} \tag{7}$$

The computation of K_{z0} is performed using similarity theory assumptions[6]. The value β is given by

$$\beta = \frac{1}{H_e}\int_0^{H_e}\beta_z(z)dz \tag{8}$$

where

$$\beta_z(z) = \frac{z}{K_z}\frac{\partial K_z}{\partial z} \quad \text{if } z \le H^* \tag{9a}$$

$$\beta_z(z) = 0 \quad \text{if } z > H^* \tag{9b}$$

where H^* is a user-specified height which represents the level above which K_z can be assumed constant with height. The functions $\beta_z(z)$ are obtained from Equation 9a using the analytical profile $K_z(z)$ corresponding to the current atmospheric stability condition.

The Output of the Model

The model can handle multiple sources and multiple receptors, simulating time-varying conditions in which each time interval (e.g., 1 hour) is treated as a stationary case. In order to correctly apply Equation 5, each source-receptor evaluation requires a horizontal rotation of the x,y coordi-

Table I. Statistical comparison of measured, C_m, and computed, C_c, hourly mean concentrations at each arc during four days of May 1980. Averages are indicated by $\overline{C}$, standard deviations by σ, correlation coefficient by r; I_r is the 95% confidence interval for r. The number of data (i.e., the number of couples C_m, C_c) is given by the number of hours multiplied by six, since concentrations are measured at six arcs downwind from the source.

	May 7	May 8	May 9	May 10	All
Number of data	54	48	12	36	150
$\overline{C_m}$	26.6	24.9	19.4	21.6	24.3
$\overline{C_c}$	25.0	29.8	16.9	19.3	24.5
σC_m	19.0	15.5	8.2	11.0	15.7
σC_c	11.1	14.8	10.0	11.4	13.2
$\overline{\lvert C_m - C_c \rvert}$	12.4	11.0	9.9	8.6	10.8
$\sigma(C_m - C_c)$	15.6	13.8	13.7	11.3	14.3
$r_{m,c}$	0.57	0.58	−0.13	0.49	0.52
I_r	(0.35, 0.71)	(0.28, 0.75)	(−0.62, 0.46)	(0.19, 0.70)	(0.39, 0.63)

nates so that the x-axis is always coincident with the wind flow at that source's effective height H_e.

The model output is a statistical summary of the concentrations computed at each receptor, during each time step, and due to each source. Partial and total concentrations are computed for hourly and multi-hour averages. Highest and highest-second-highest values are also evaluated.

Preliminary Model Evaluation

The methodology proposed above has been successfully tested[8] by comparison with finite-difference numerical solutions of the K-theory equation, using several theoretical $u(z)$ and $K_z(z)$ profiles from literature data. The KAPPA-G model, therefore, is capable of approximating even complex vertical profiles well using power laws. It is true that a power law profile for $K_z(z)$ cannot be considered a fully appropriate choice, since it cannot satisfy the condition $K_z(z) \rightarrow \sim 0$ as $z \rightarrow H$, that would be required[9] to realistically represent the behavior of vertical diffusion at the top of the boundary layer. Nevertheless, numerical tests have shown that, at least for ground level receptors, a power law function for $K_z(z)$ provides an adequate approximation.

Comparison between Model Outputs and SF_6 Tracer Data

This section presents an actual test of the model, using SF_6 data from tracer experiments[10] conducted by the Electric Power Research Institute, EPRI (File No. 3 in the EPRI data base, data from the week beginning 5 May 1980).

The tracer experiments[10] were performed as part of the flat terrain measurement program of the EPRI Plume Model Validation and Development (PMV&D) Project. The selected site was the Kincaid Generating Station of the Commonwealth Edison Company (CECO) located in central Illinois, a flat, isolated agricultural area. The EPRI PMV&D project has been designed to 1) provide a good description of elevated buoyant plume dynamics; 2) evaluate the simulation performance of plume models and model components; and 3) develop more refined mathematical models and numerical methodologies for plume simulation.

The comparison presented below between KAPPA-G model outputs and SF_6 tracer data is a preliminary one, aiming at a qualitative understanding of the level of performance that can be expected from the model. A full model evaluation exercise is expected to be performed soon.

This test has been conducted using the model KAPPA-G, as described in the previous section, with the following further assumptions and parameterizations:

1. The meteorological input was inferred from observations recorded at one meteorological station (the Central Station).
2. Wind speed and direction were taken at 30 m (the same wind speed was also used to evaluate K_{z0} at 30 m).
3. The Monin-Obukhov length L was evaluated[11] from the bulk Richardson number measured using the wind speed u at 10 m, and the temperature difference, ΔT, between 2 m and 10 m.
4. The value of the roughness length z_0 was taken equal to 0.1 m (which is typical of farmland with few buildings).
5. The PG atmospheric stability was used for evaluating σ_y according to the Briggs open country formulas.
6. The parameter β was assumed equal to 1, in unstable conditions, and $(1 - \alpha)$ in neutral conditions.
7. The parameter α was computed using only the wind speed measured at 30 m (i.e., theoretical profiles were used).

The above assumptions and parameterizations were used for all the KAPPA-G simulations without any "tuning."

A four-day period totaling 25 hours was modeled. In this preliminary semiquantitative performance evaluation, the following concentration values were selected for comparison at each hour:

a. The average cross-wind integrated concentration (measured and computed); i.e., the average concentration at all receptors of a given arc (each arc contains all the receptors at approximately the same downwind distance from the SF_6 source).
b. The maximum concentration (measured and computed)

Table II. Statistical comparison of maximum hourly concentration data at each arc (same symbols as in Table I).

	May 7	May 8	May 9	May 10	All
Number of data	54	48	12	36	150
$\overline{C_m}$	75.7	74.7	54.2	88.7	76.8
$\overline{C_c}$	86.7	104.4	65.9	82.2	89.6
σC_m	59.8	52.3	22.8	43.9	52.4
σC_c	36.4	42.4	33.5	41.1	41.0
$\overline{\lvert C_m - C_c \rvert}$	47.5	40.7	37.0	32.1	40.8
$\sigma(C_m - C_c)$	58.0	39.9	44.0	41.1	49.6
$r_{m,c}$	0.35	0.66	−0.19	0.53	0.46
I_r	(0.09, 0.59)	(0.48, 0.78)	(−0.66, 0.41)	(0.23, 0.72)	(0.32, 0.62)

among all receptors of a given arc (even if at different receptors).

The results are summarized in Tables I and II, which quantify the average performance of the model, and in Figures 1 through 4 which show specific simulation examples. Table I shows a statistical summary of the comparison of the above Data a, while Table II shows the same summary for the above Data b. In addition, Figures 1 and 2 show the downwind variation of the concentration field (Data a average, and Data b maximum) during two selected hours, respectively; while Figures 3 and 4 present the temporal variation, at two selected arcs, respectively, of the concentration values (average and maximum) during two different simulation days.

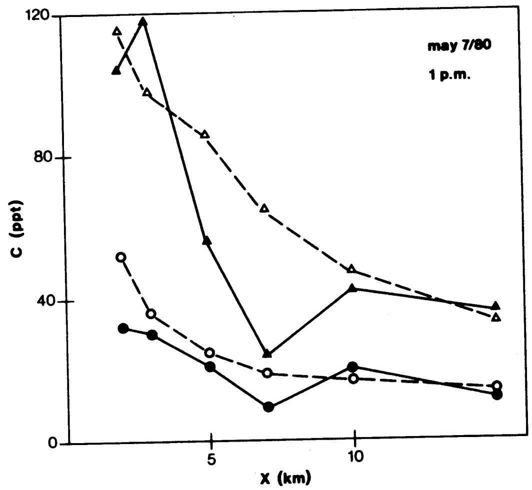

Figure 1. Downwind variation (i.e., at six arcs) of the average concentration (circles) and the maximum concentration (triangles). In this figure and in the following ones, measured values are indicated by solid lines; computed values by dotted lines.

Results show a clear ability of the model to provide simulations with little bias with respect to actual measurements. Both Table I and Table II, in fact, show that average computed $\overline{C}_c$ concentrations are quite close to the measured $\overline{C}_m$ ones. Concentration plots in Figures 1 through 4 illustrate a simulation behavior which is qualitatively correct even though occasional large errors are present.

If we consider the generally poor performance currently achieved by both simple and complex diffusion models for short-term (e.g., hourly) simulations, the results presented in these tables and figures are encouraging. Correlation coefficients are quite low but, nevertheless, both average concentration data and average maxima are very close to the simulated values. The average concentration error is about one-half of the value itself, showing that most simulation outputs are within a factor of two of the actual measured concentration data.

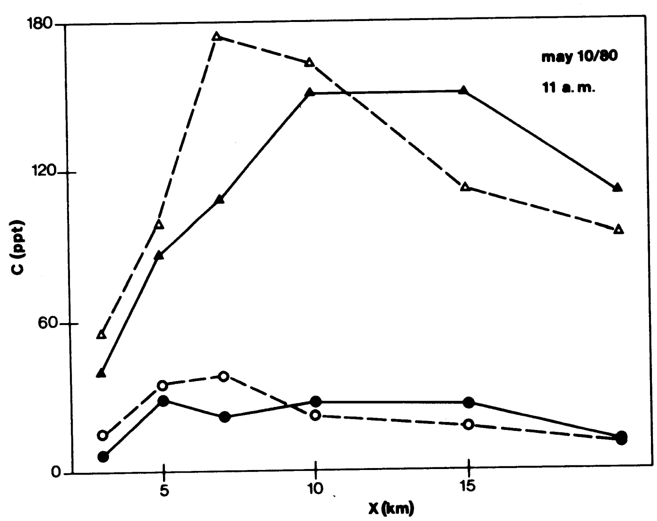

Figure 2. Downwind variation of the average concentration (circles) and the maximum concentration (triangles).

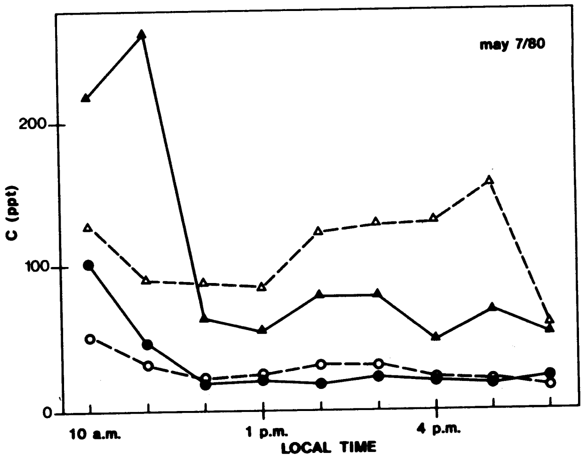

Figure 3. Temporal variation in the daytime of the average concentration (circles) and the maximum concentration (triangles) at the arc at 5 km from the source.

Conclusions and Future Developments

This preliminary evaluation has provided interesting results which confirm, in our opinion, the potential suitability of this approach as an alternative to the Gaussian equation. Certainly, much effort is still required to improve the model parameterization and fully evaluate its actual performance. We expect further improvements in model parameterization will result from the full comparison with SF_6 tracer data which is now in progress.

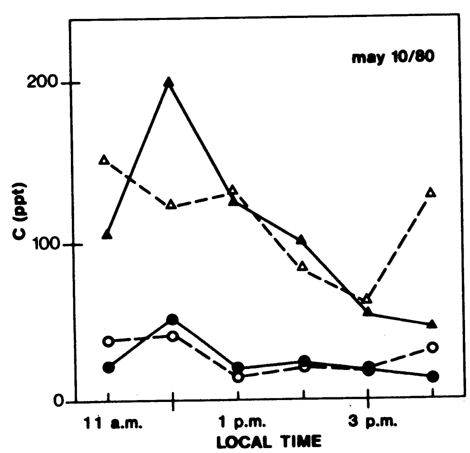

Figure 4. Temporal variation in the daytime of the average concentration (circles) and the maximum concentration (triangles) at the arc at 7 km from the source.

Another interesting future application of the model KAPPA-G is in climatological simulations. Until now, the only climatological application of dispersion models has been made using Gaussian algorithms for long-term (e.g., annual) simulations.[12] The KAPPA-G approach allows more refined representation of vertical diffusion, still maintaining a steady-state explicit formulation. Therefore, it can be easily incorporated into a climatological model, using the measured frequency distribution of the major meteorological parameters (such as wind speed, direction, and stability) for long-term air quality simulations.

Acknowledgments

The authors express their gratitude to Ms. Roberta Lewis and Dr. Ivar Tombach of AeroVironment Inc., for their useful editorial review of the manuscript. Appreciation is extended to Ms. Shirley Bauer for her typing of the manuscript. This work has been partially sponsored by the "Progetto Finalizzato Energetica II" of the Italian CNR (Center for National Research).

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This technical paper was submitted for peer review July 17, 1985; the revised manuscript was received January 30, 1986.