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EVALUATION OF A DISPERSION MODEL BASED ON A NON-GAUSSIAN ANALYTICAL SOLUTION IN TURBULENT SHEAR FLOW.

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ABSTRACT

The paper presents a mixed methodology,for the simulation of atmospheric diffusion,in which vertical diffusion is computed using the analytical solution of the K-theory equation,while horizontal diffusion is simulated by the Gaussian formula. The performance of this approach is evaluated by comparison with SF_6 tracer data collected by EPRI.

1. INTRODUCTION AND SUMMARY

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 non-homogeneous conditions on a three-dimensional domain. The K-theory can virtually accept any complex three-dimensional meteorological input,but generally requires a finite-difference numerical integration which is computationally expensive and,sometimes,affected by numerical advection errors.

However,the K-theory equation can be analytically solved in two dimensions under the following simplifying assumptions (Yeh and Huang, 1975;Demuth,1978):

1.- dispersion in steady-state transport conditions;

2.- horizontal wind,u,expressed as a power law function of height;

3.- vertical eddy diffusion coefficient, K_z, expressed as a power law function of height.

Roberts (see Calder,1949) obtained this two-dimensional solution for ground level sources. Smith (1957) found a solution for elevated sources with u and K_z profiles following Schmidt's coniugate law. Rounds (1955) proposed a more general solution which,however,turned out to be valid only for linear profiles of K_z. Finally,Yeh and Huang (1975) and Demuth (1978) obtained a more general analytical solution. We have adopted this latter solution for the development of our package,KGAUSS,which allows the performance of a three-dimensional steady-state simulation using the Gaussian formula for the treatment of horizontal diffusion (as proposed by Huang,1979). We suggest that,in many applications,this approach can be used,instead of the Gaussian formula,for taking a better account of the vertical stratification of the atmosphere and,expecially,of the wind shear.

The rest of this paper presents in section 2 a detailed description of the proposed model,together with its parametrizations and working options. Section 3 shows a preliminary performance evaluation of the model using some of the SF_6 tracer data collected during the EPRI experiment at Kincaid,Ill. (file 3,data for week beginning 5 May 1980). Finally,section 4 presents conclusions,recommandations and possible future developments.

2. THE KGAUSS PACKAGE

The computer package KGAUSS is written in standard FORTRAN language and can be virtually installed in any computer. This package performs steady-state simulations of atmospheric diffusion phenomena under the assumptions and parametrizations described below.

2.1.-<u>The analytical solution of the K-theory equation.</u>

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

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

with initial condition

$$C \rightarrow \frac{Q}{u_s} \delta (z - H_s) \, \delta (y) \qquad \text{as } x \longrightarrow 0$$

and boundary conditions

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

where C (x,y,z) is the mean concentration field, Q is the emission rate of the source in $(0,0,H_s)$, H_s is the effective height of the source, H is the height of the mixing layer, and $\delta(\ldots.)$ means the delta function, while the subscript "s" means "at the source location". Under the conditions

$$u = u(z) = u_o \, (z/h_o)^{\alpha} \qquad (2a)$$

$$K_z = K_z(z) = K_{zo} \, (z/h_o)^{\beta} \qquad (2b)$$

$$K_y = u * (\text{ any function of } x) \qquad (2c)$$

$$H = + \infty$$

and

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

where h_o is the height where u_o and K_{zo} are evaluated, the solution of (1) for ground level concentration (g.l.c.) is (Yeh and Huang, 1975):

$$\overline{C} \, (x,0) = \frac{Q}{\delta^{\eta}} \; \frac{1}{\Gamma(\gamma)} \; \frac{h_o^{\eta}}{u_o^{\nu} \, (x \, K_{zo})^{\gamma}} \; \exp \left[- \frac{u_o \, h_o^{\beta} \, H_s^{\delta}}{h_o^{\alpha} \, \delta^2 \, K_{zo} \, x} \right] \qquad (3a)$$

where:

$\delta = \alpha - \beta + 2$

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

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

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

and Γ denotes the Gamma function.

Under the same conditions (2), but with $H < +\infty$, the solution of Eq.(1) is (Demuth, 1978):

$$\overline{C}(x,0) = \frac{2\,Q\,q\,h_o^{\alpha}}{H^{\alpha+1}\,u_o}\left\{\gamma + R^p \sum_{1}^{\infty}{}_i \frac{J_{\gamma-1}(\sigma_{\gamma i}\,R^p)\,\sigma_{\gamma i}^{\gamma-1}}{\Gamma(\gamma)\,J_{\gamma-1}^2\,\sigma_{\gamma i}\,2^{\gamma-1}}\ \exp\left|-\frac{\sigma_{\gamma i}^2\,q^2\,K_{zo}\,x}{H^{\delta}\,h_o^{r}\,u_o}\right|\right\} \qquad (4a)$$

where:

$R = H_s / H$

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

$q = \delta/2$

$r = \beta - \alpha$

and J_γ represents the modified Bessel function of the first kind and order γ and $\sigma_{\gamma i}$, $i = 1, 2, \ldots\ldots$, are the zeros of J_γ.

The solution of Eq.(1) for concentrations above the ground is, for $H = +\infty$,

$$\overline{C}(x,z) = \frac{Q\,(z\,H_s)^{p}\,h_o^{\beta}}{\delta\,K_{zo}\,x}\,\exp\left(-\frac{u_o\,h_o^{r}(z^{\delta} + H_s^{\delta})}{\delta^2 K_{zo}\,x}\right)\,I_{-\nu}\left(\frac{2\,u_o\,h_o^{r}(z\,H_s)^q}{\delta^2\,K_{zo}\,x}\right) \qquad (3b)$$

and, for $H < +\infty$

$$\overline{C}(x,z) = \frac{2\,Q\,q\,h_o^{\alpha}}{H^{\alpha+1}\,u_o}\left\{\gamma + \left(\frac{z\,R}{H}\right)^{p} \sum_{1}^{\infty}{}_i \frac{J_{\gamma-1}(\sigma_{\gamma i}\,R^q)\,J_{\gamma-1}(\sigma_{\gamma i}(z/H)^q)}{J_{\gamma-1}^2(\sigma_{\gamma i})}\ \exp\left(-\frac{\sigma_{\gamma i}^2\,q^2 K_{zo}\,x}{H^{\delta}\,h_o^{r}\,u_o}\right)\right\} \qquad (4b)$$

If σ_y^2 represents the mean square particle displacement along the cross-wind direction (y-axis), with the condition

$$\frac{1}{2} \frac{d}{d\,x} \sigma_y^2 = \frac{1}{u} K_y$$

then, in (3) , (4) the lateral diffusion can be described by a Gaussian-type term which gives the final three-dimensional formula used in the KGAUSS package:

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

2.2 The plume rise

The package utilizes the Briggs' formulas (Briggs,1971 and 1975) for the computation of the dynamic plume rise $\Delta h(x)$.

2.3 The definition of the model's input

The package is very flexible in the definition of the meteorological input. The minimum information required, besides the emission information, is:

1.-the wind speed measured at a certain height;

2.-the vertical atmospheric stability (either a Pasquill-Gifford stability class (PG) or the Monin-Obukhov length);

3.-the horizontal atmospheric stability (either a PG stability or the standard deviation of the horizontal wind direction).

The package utilizes this minimum information for the computation, by theoretical extrapolation, of full vertical profiles. However, if vertical meteorological profiles are available, they can be directly used in the package, thus avoiding the above extrapolation.

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

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

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

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

$$\alpha = (u_p(H_s) - \bar{u})/\bar{u} \tag{7}$$

The computation of K_{zo} and β is performed in the following way. K_{zo} is computed using similarity theory assumptions(Huang,1979). The value β is given by

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

where

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

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

where H* is a height specified as an input parameter,and represents the height above which the K_z values can be assumed constant. The values $\beta_z(z)$ are taken from the analytical theoretical profiles presented by Huang (1979).

2.4 The output of the model

The model can handle multiple sources and multiple receptors for time-varying simulations in which each time interval (e.g., 1 hour) is treated as a stationary case. In order to perform this computation,the model translates and rotates the coordinate system for satisfying,for each source,the geometry required by the rotation described in section 2.1.

The model output is the concentration computed at each receptor,during each time step,due to each source.

3. COMPARISON BETWEEN MODEL OUTPUTS AND EPRI SF_6 TRACER DATA

The proposed methodology had been succesfully tested (Tirabassi et al.,1982) by comparison with finite-difference solutions of the K-theory equation. These finite-difference solutions were obtained using several theoretical u and K_z profiles found in the literature, and therefore KGAUSS showed its capability of well approximating these profiles with power laws.

This section is presenting an actual test of the model,using SF_6 data from EPRI field experiments (File #3, data from week beginning 5 May 1980). This comparison is a preliminary one,aiming at a qualitative understanding of the level of performance that can be expected from this approach. A full model evaluation exercise,following EPA recommendations,is expected to be soon performed.

This comparison has been performed using the model,as described in section 2, with the following assumptions and parametrizations:
1.-the meteorological input was inferred from the Central Station

Meteorological observations;

2.-wind speed and direction were taken at 30 m (this wind speed was also used to evaluate K_{zo} at 30 m) ;

3.-the Monin-Obukhov length was evaluated (Wang,1981) from the bulk Richardson number measured from u at 10 m,and the temperature difference,ΔT,at 2 m and 10 m;

4.-the value of z_o was taken equal to 0.1 m;

5.-the PG atmospheric stability was used for evaluating σ_y with the Briggs open country formulas.

6.-the parameter β was assumed equal to 1.,in unstable conditions, and (1.- α) in neutral conditions.

7.-the parameter α was computed using only the single value of u at 30 m (theoretical profiles).

All the above assumptions and parametrizations were used for all the simulations of KGAUSS without any "tuning".

The model was applied during four days for a total of 25 hours. In this preliminary semi-quantitative performance evaluation,the following concentration values were selected for comparison at each hour:

1.- the average concentration (measured and computed) in all receptors of a given arc (arcs are at different downwind distances from the SF_6 source);

2.- the maximum concentration (measured and computed) among all receptors of a given arc (even if in different receptors).

Table 1 shows a statistical summary of the comparison of the above data 1.,while Table 2 shows the same summary for the above data 2.. In addition,Figures 1 and 2 show the spatial variation of the concentration field (data 1. and 2. above) during two selected hours;and Figures 3 and 4 present the temporal variation at a selected arc of the

Table 1.- Statistics of average hourly concentration data at each arc (C_m, measured; C_c, computed): averages $\overline{C}$, standard deviations σ_C, correlation coefficient r, 95% confidence interval for r I_r.

	#1	#2	#3	#4	ALL
N of hours	9	8	2	6	25
$\overline{C}_m$	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
$r_{m,c}$	.57	.58	-.13	.49	.52
I_r	(.35,.71)	(.28,.75)	(-.62,.46)	(.19,.70)	(.39,.63)

Table 2.- Statistics of maximum hourly concentration data at each arc (C_m, measured; C_c, computed; as Table 1.).

	#1	#2	#3	#4	ALL
N of hours	9	8	2	6	25
$\overline{C}_m$	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
$r_{m,c}$	.35	.66	-.19	.53	.46
I_r	(.09,.59)	(.48,.78)	(-.66,.41)	(.23,.72)	(.32,.62)

concentration data (1. and 2.,above) during two full days of simulation. The tables quantify the average performance of the model,while the figures show two examples of simulation.

4. CONCLUSIONS AND FUTURE DEVELOPMENTS

This preliminary evaluation has provided interesting results which confirm,in our opinion,the suitability of this approach as an alternative procedure instead of the Gaussian equation. Certainly,much effort is still required for improving the model parametrization and fully evaluating its actual performance. We expect further improvements in model parametrization to be obtained from the full comparison with SF_6 tracer data which is under progress.

In addition,we plan to use the KGAUSS approach in an effort to improve climatological air quality simulations that,until now, have been performed only with Gaussian formulas.

FIGURE CAPTIONS

Fig. 1.- Spatial variation of the average concentration field (circles) at different arcs (downwind distances) and of the maximum concentration values (triangles)(measured:solid lines; computed:dotted lines).

Fig. 2.- Spatial variation of the average concentration field (circles) at different arcs (downwind distances) and of the maximum concentration values (triangles)(measured:solid lines; computed:dotted lines).

Fig. 3.- Temporal variation in the daytime of the average concentration field (circles) and the maximum concentration values (triangles) (measured:solid lines; computed:dotted lines).

Fig. 4.- Temporal variation in the daytime of the average concentration field (circles) and the maximum concentration values (triangles) (measured:solid lines; computed:dotted lines).

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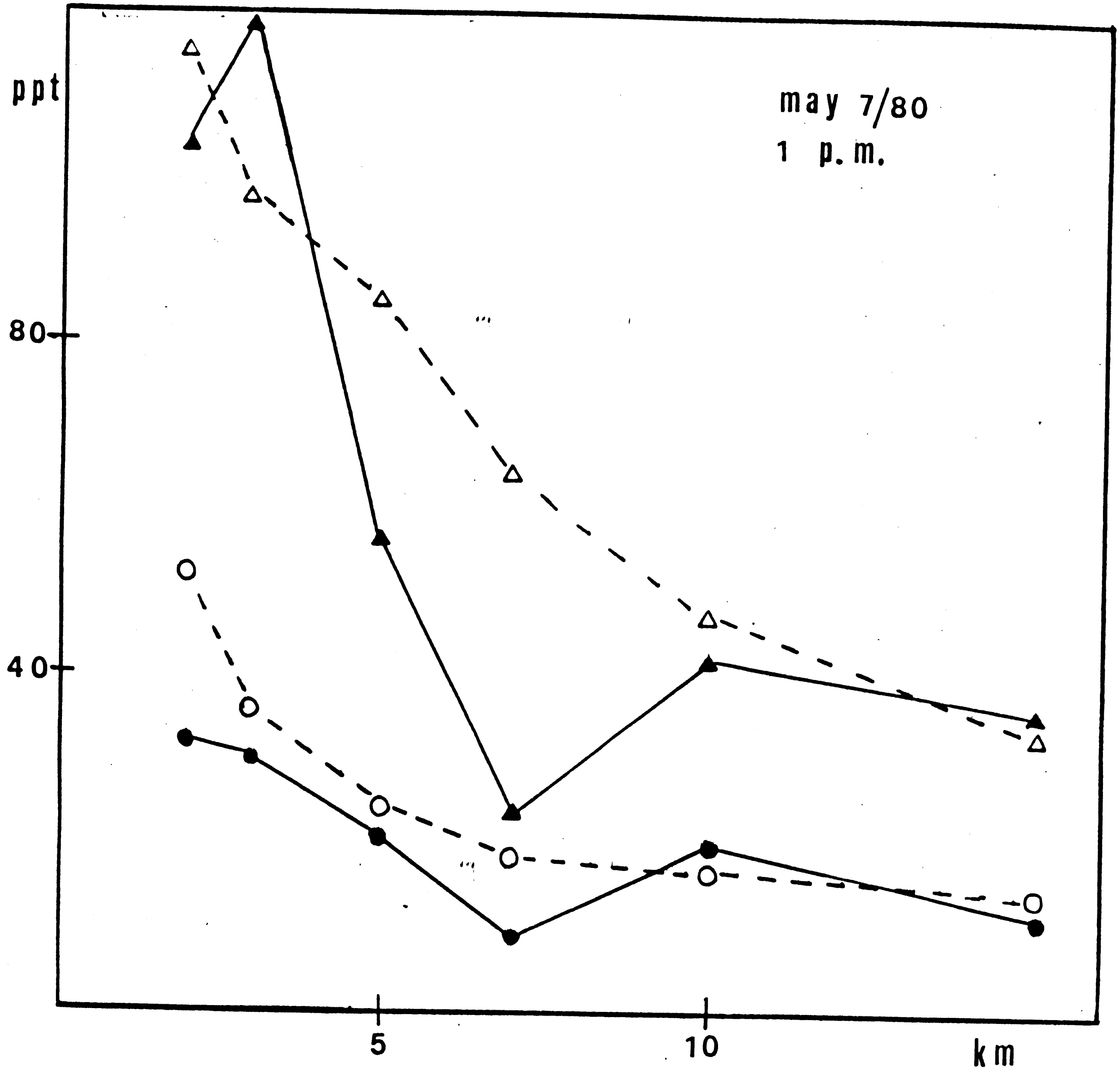

Fig. 1

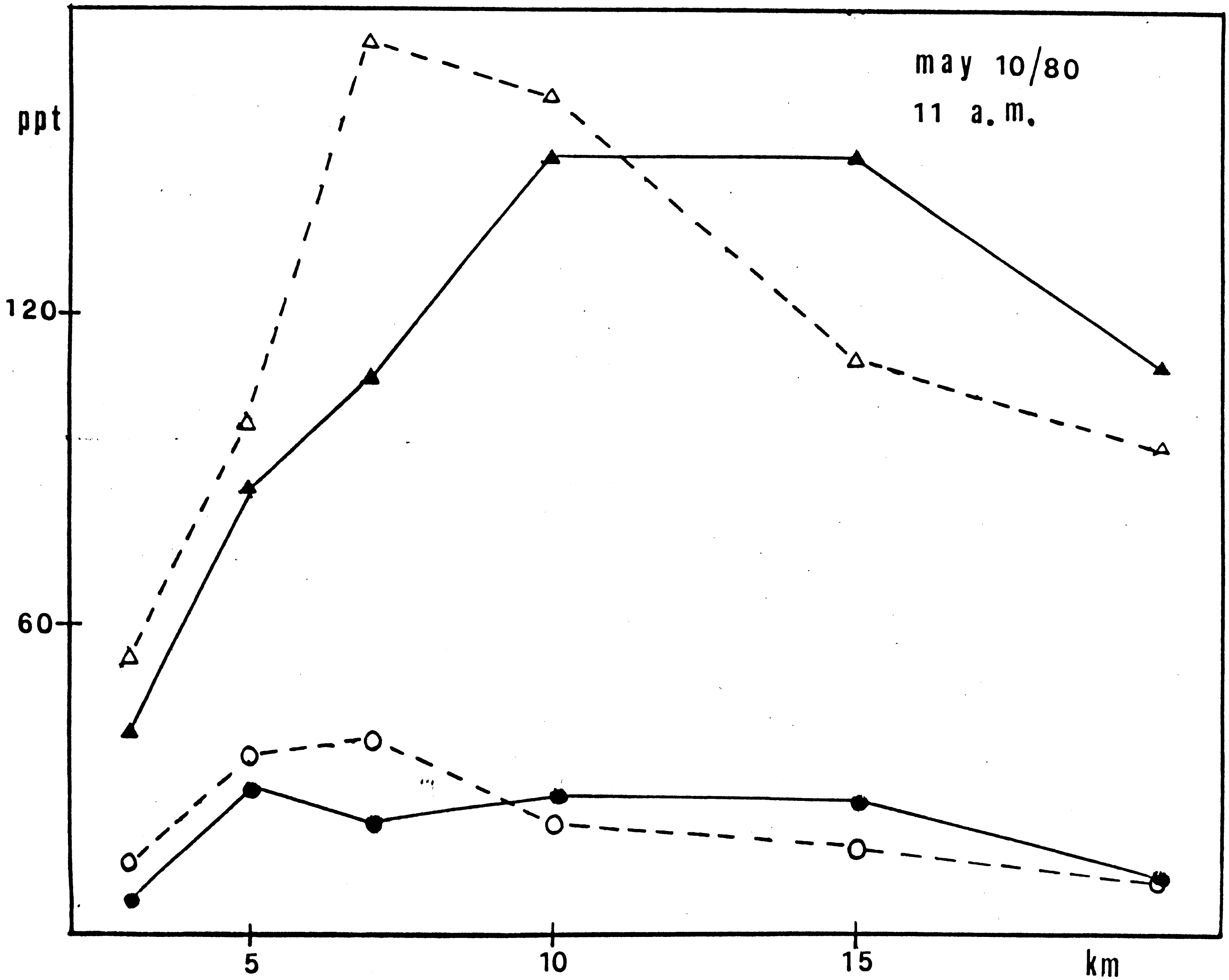

Fig. 2

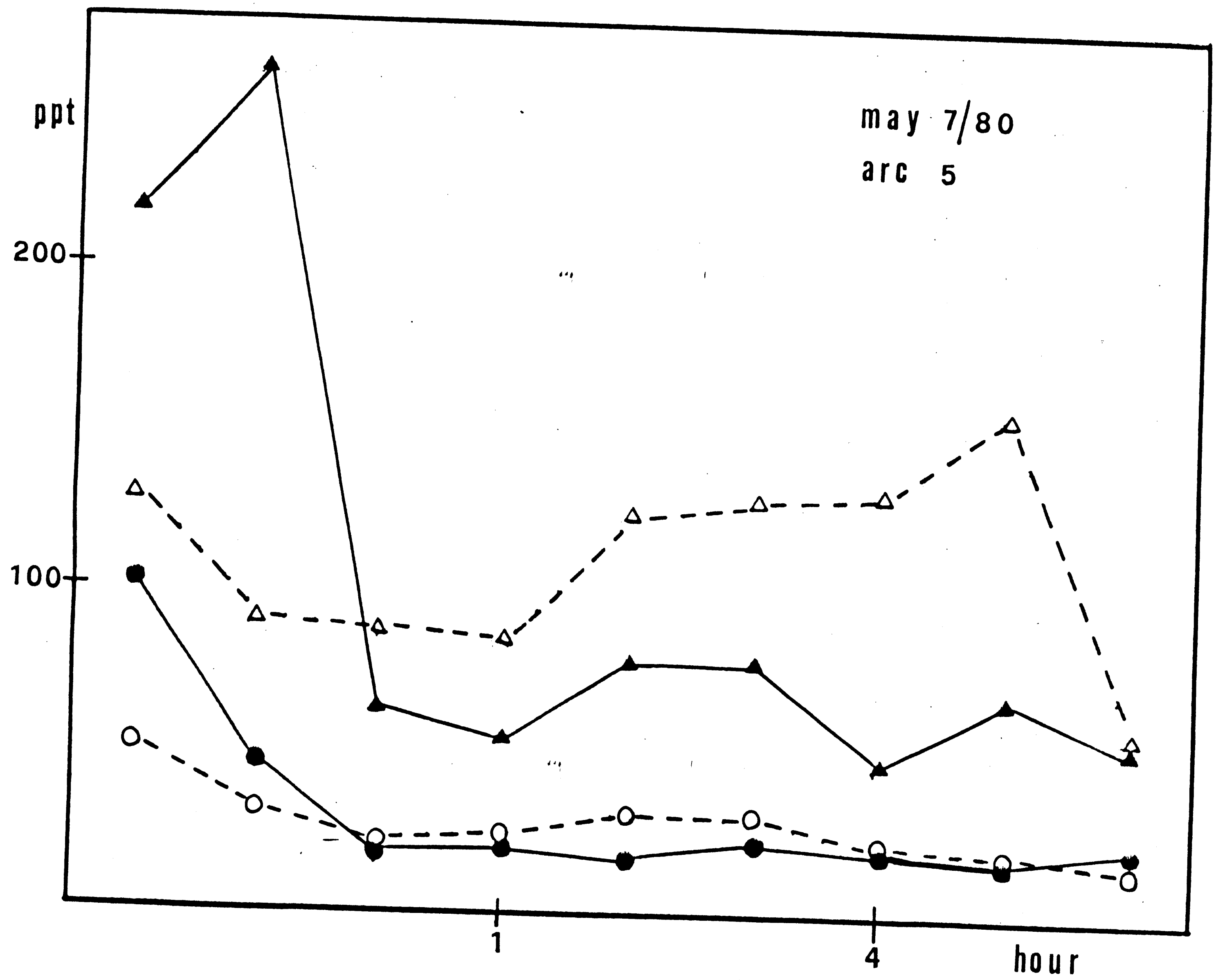

Fig. 3

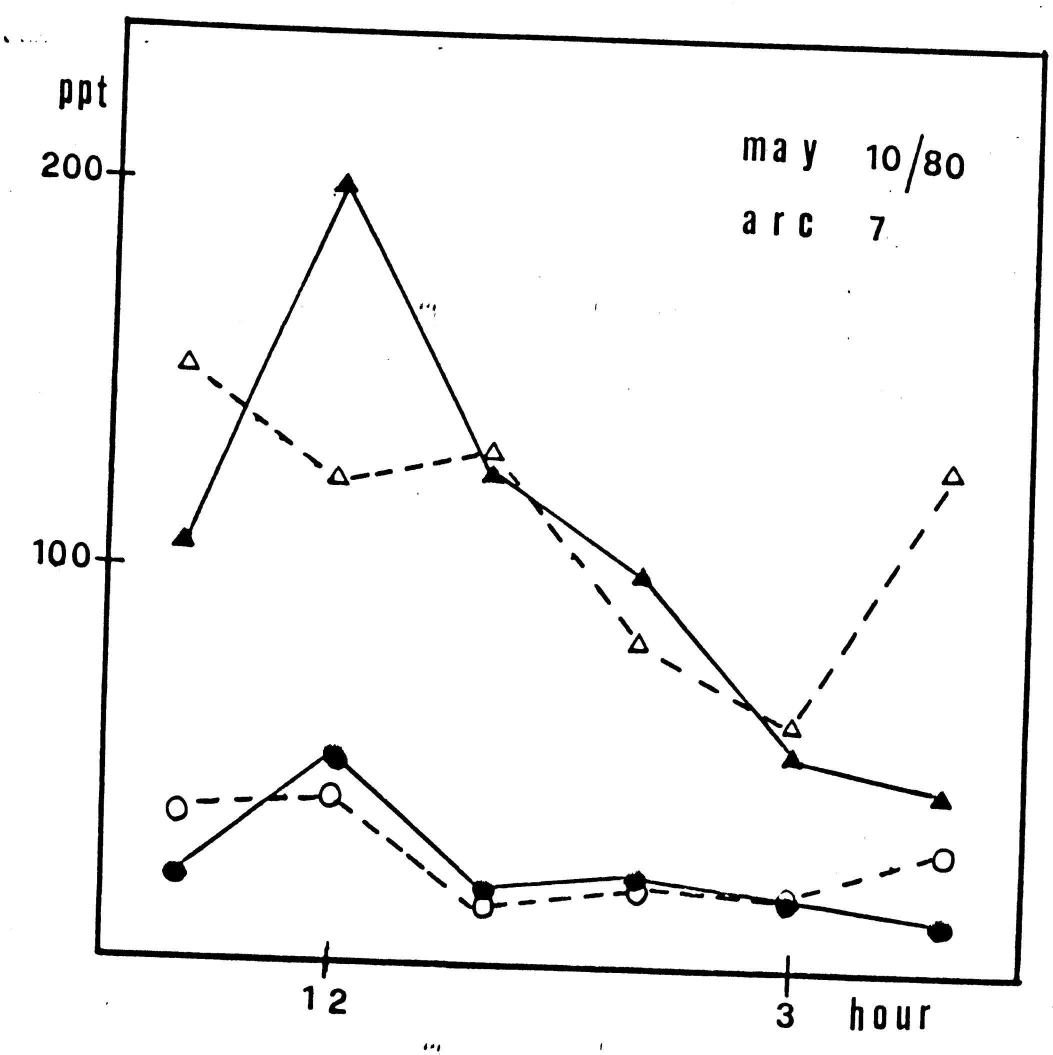

Fig. 4