

A numerical solution for dispersal of air pollutants

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(Received 4 September 1979)

ABSTRACT. The dispersal of pollutants from an elevated point source was computed by a numerical method. The computations were made with forward time differences. But backward space differences were used for computing the horizontal advection of pollutants. As eddy diffusivity, which varied with altitude (Z), was used in the numerical computations. The results were compared with a Gaussian plume, and it was observed that the latter did not provide correct estimates at larger distances downstream, because it neglected the horizontal advection of pollutants. The paper presents a comparison between a numerical solution of the diffusion equation, and a Gaussian plume model, for different atmospheric conditions.

1. Introduction

Many computations have been made in the past by assuming a Gaussian distribution for the pollutants that emanate from an industrial stack (Passquill, 1962). But, as we can see, the distribution need not be Gaussian because the pollutants could be horizontally advected by the prevailing wind. The wind and eddy diffusivity also vary with height. The purpose of the paper is, therefore, to compute downstream concentrations by a numerical solution of the diffusion equation, and to compare the results with a Gaussian distribution.

2. Basic equations

The diffusion of pollutants is governed by

$$\frac{dC}{dt} = \nabla \cdot (K \nabla C) \quad (2.1)$$

where, C is the pollutant concentration in micrograms per cubic metre, K is the coefficient of eddy diffusivity ($\text{m}^2 \text{sec}^{-1}$) and ∇ is the del operator in three dimensions. If we consider only horizontal advection and neglect the downwind (x) or cross-wind (y) components of diffusion, we have

$$C_t + u(Z) C_x = (K C_z)_z \quad (2.2)$$

where the subscripts denote partial derivatives. We justify the neglect of horizontal diffusion by not considering very small values of wind velocity, *i.e.*, calm condition etc Eqn. (2.2) will be solved for the positive half of the X axis [$0 < x < \infty$].

3. Initial and boundary conditions

An appropriate initial condition is to ensure that at $t=0$, the region is not polluted. We put

$$C(x, Z, 0) = 0 \quad (3.1)$$

The upper and lower boundary conditions specify no flux across the earth's surface ($Z=0$), and the base ($Z=H$) of an upper inversion. Thus

$$K(Z) \frac{\partial C}{\partial Z} = 0 \quad (3.2)$$

The mixing depth is roughly estimated to be 400 m during winter season in northwest India and the data on continuous measurement for mixing depth is not available.

When the above boundary conditions are suddenly imposed, very high values of flux were created near the upper and lower boundary (Carslaw and Jaeger 1976). As the upper and lower boundary conditions were reflective, this soon lead to unrealistic values within the range of interest. To overcome this difficulty, the integration was started with a Gaussian plume for the first four time steps. This was the time taken for the plume dimension to become comparable to the size of the unit vertical grid. We put

$$C_0(x, Z, t) = \frac{Q}{2\pi u \sigma_y \sigma_z} \exp^{-1/2} [(Z - \bar{h}/\sigma_z)^2 + (Z + \bar{h}/\sigma_z)^2] \quad (3.3)$$

for $t \leq t_1$ and $\sigma_z \leq \Delta Z$

$$C(0, Z, t) = C_0$$

$$\text{for } t > t_1 \quad (3.4)$$

σ_y and σ_z represent the standard deviation of pollutants in the cross-wind and vertical direction, while Q is the rate of emission ($\mu\text{g Sec}^{-1}$) from the stack. The effective stack height (h) was taken to be the sum of the physical height of the stack and the plume ascent on account of buoyancy. The initial conditions represented by (3.3) and (3.4) were different from that of Runca and Sardei (1975), who used a step function for this purpose.

It is worth mentioning here that Dirac delta function, *i.e.*, $\delta(z-h)$ has also been used instead of the Eqn. (3.4) for computing $C(0, Z, t)$ but the results yielded by the Eqn. (3.4) are better.

4. Numerical method

One of several differencing schemes could be used for numerical integration. Let

$$t = n\Delta t \tag{4.1.a}$$

$$x = j\Delta x \tag{4.1.b}$$

$$Z = l\Delta Z \tag{4.1.c}$$

We considered forward time and backward space differences for advection, whence

$$C_t = (C^{n+1} - C^n) / \Delta t \tag{4.2.a}$$

$$u(Z) C_x = u(Z) (C_j - C_{j-1}) \Delta x \tag{4.2.b}$$

The advection part of the scheme is stable if $u\Delta T / \Delta x < 1$

Finite differences for computing vertical diffusion are shown in Fig 1. To compute the vertical diffusion at A for example, we first calculated the fluxes at B and C. The eddy diffusivity at B and C were obtained by averaging the values immediately above and below. Thus,

$$K_B = 1/2(K_{l+1} + K_l)$$

$$K_C = 1/2(K_l + K_{l-1})$$

Where K_B and K_C represent the diffusivity at B and C. Similarly, the fluxes at B and C were

$$F_B = K_B \left(\frac{\partial C}{\partial Z} \right)_B = K_B (C_{l+1} - C_l) / \Delta Z$$

$$F_C = K_C \left(\frac{\partial C}{\partial Z} \right)_C = K_C (C_l - C_{l-1}) / \Delta Z$$

Whence, the vertical diffusion at A was

$$\frac{\partial}{\partial Z} \left(K \frac{\partial C}{\partial Z} \right)_A = (F_B - F_C) / \Delta Z$$

If we leave out the advection term in 2.2, then the remaining equation is the familiar diffusion equation with Z and t as independent variables. For computational stability, we placed the restriction $K\Delta t / (\Delta Z)^2 \leq 0.5$ (Richtmyer and Morton 1967).

This meant using different values of Δt for different stability conditions.

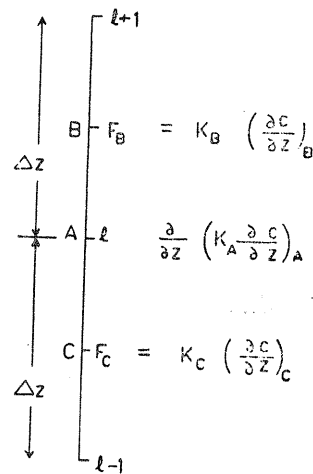


Fig. 1.

It is known that truncation errors due to horizontal advection generate a fictitious viscosity. Its magnitude may be estimated by expanding C in a Taylor series. We have

$$(C_t)_n \simeq (C^{n+1} - C^n) / \Delta t - \frac{1}{2} \Delta t (C_{tt})_n + \dots$$

$$(C_x)_j \simeq (C_j - C_{j-1}) / \Delta + \frac{1}{2} \Delta x (C_{xx})_j + \dots$$

Hence, the truncation error (E) is

$$E \simeq 1/2 (u \Delta x C_{xx} - \Delta t C_{tt})$$

But, as

$$C_{tt} \simeq u^2 C_{xx}$$

We find

$$E \simeq 1/2 u \Delta x (1 - u \Delta t / \Delta x) u C_{xx} \simeq K_H C_{xx}$$

Where K_H is the coefficient of artificial viscosity. Its magnitude is

$$K_H \simeq 1/2 u \Delta x (1 - u \Delta t / \Delta x)$$

The truncation error (E) builds up rapidly during numerical integration, and soon exceeds vertical diffusion. A method due to Mahoney and Egan (1970) was used to overcome this difficulty. This involves separating the horizontal transport and vertical diffusion in (2.2).

The vertical diffusion was first computed and stored for each grid point (j, l). At the same time, the numerical value of $u \Delta t / \Delta x$ was stored for every grid point. Whenever this exceeded 1.0 at a grid point, the pollutant was advected horizontally and the value of $u \Delta t / \Delta x$ was reset to its current value minus 1.0. This was to prevent the horizontal advection of pollution

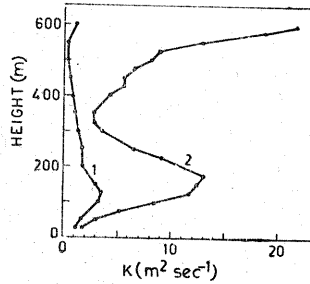


Fig. 2. Variation of eddy diffusivity K with height on a day with warm air advection (1) and with cold air advection (2) After Lettau and Hoerber (1964).

at a speed greater than u . As indicated by Mahoney and Egan (1970) this process creates minor irregularities due to recycling the value of $u \Delta t / \Delta x$, but they may be removed by averaging over four to five steps. As each time step is of 50 secs duration, there is no serious loss of detail of such averaging.

5. Data input

The following inputs were used for numerical integration :

- (i) Emission rate (Q) : 1 ton hr⁻¹
- (ii) Height of stack H_1 : 80m
- (iii) Δx : 20 m
- (iv) Δx : 1 Km
- (v) Δt : 50 secs for stable and neutral conditions and 15 secs for unstable conditions.

For this experiment we used the pasquill (1962) and Turner (1964) classification of atmospheric stability. This classification is based on (i) wind speed, (ii) cloud cover and (iii) solar insolation, and it contains 7 categories of stability. The details are given in Appendix 1.

The variation of eddy diffusivity with stability and height was obtained from the results of Lettau and Hoerber (1964). This is shown in Fig. 2. Lettau and Hoerber provided the variation of K with Z for stable and unstable conditions. We obtained the variation for neutral stability by interpolation between curves (1) and (2) of Fig. 2.

A power law was assumed to determine the vertical profile of $U(z)$. We have

$$u = u_1(Z/Z_1)^p$$

Where u, u_1 represent the wind speed at Z and Z_1

TABLE 1

Variation of σ_y and σ_z

Stability Category	σ_y (m)	σ_z (m)
A	$\cdot 22X/(1+X \times 10^{-4})^{1/2}$	$\cdot 20X$
B	$\cdot 16X/(1+X \times 10^{-4})^{1/2}$	$\cdot 12X$
C	$\cdot 11X/(1+X \times 10^{-4})^{1/2}$	$\cdot 08X/(1+X \times 2 \times 10^{-4})^{1/2}$
D	$\cdot 08X/(1+X \times 10^{-4})^{1/2}$	$\cdot 06X/(1+X \times 15 \times 10^{-4})^{1/2}$
E	$\cdot 06X/(1+X \times 10^{-4})^{1/2}$	$\cdot 03X/(1+X \times 3 \times 10^{-4})$
F	$\cdot 04X/(1+X \times 10^{-4})^{1/2}$	$\cdot 01X/(1+X \times 3 \times 10^{-4})$

The values of p were 1/9, 1/7 and 1/3 for unstable, neutral and stable conditions.

σ_y and σ_z depend on the downstream distance in addition to the stability of the atmosphere. We used following expressions, due to Briggs (Gifford 1976) in our work.

Following Moore (1974), the expression for plume rise were

1. Unstable/neutral : $\Delta h = \frac{60+5H}{u} Q_H^{0.25}$
2. Stable and weak wind : $\Delta h = \frac{116}{u} Q_H^{0.25}$
3. Stable and strong wind : $\Delta h = \frac{160}{u} Q_H^{0.25}$

Q_H stands for rate of heat emission. We used a constant value of 25.6 mega watts in our computations.

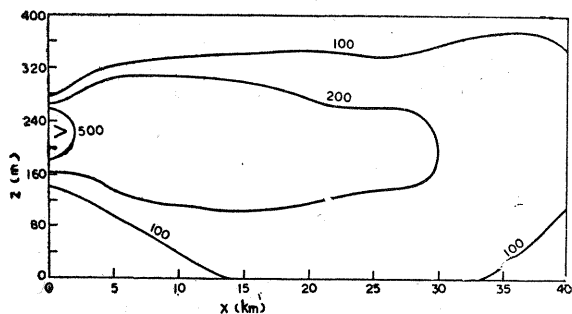


Fig. 3.

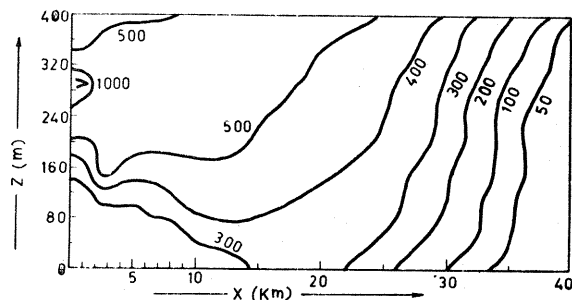


Fig. 4.

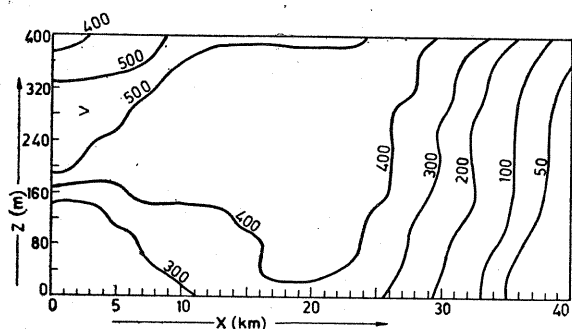


Fig. 5.

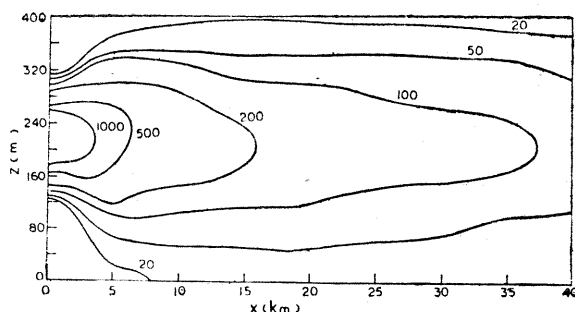


Fig. 6.

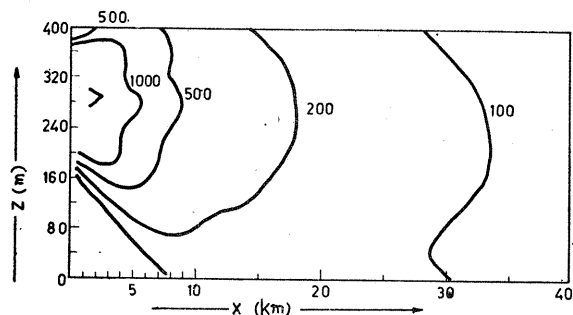


Fig. 7.

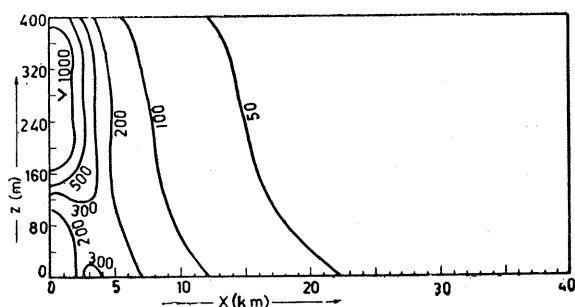


Fig. 8.

6. Results

In Figs. 3, 4 and 5 we depict the pollution concentrations after 5 hours of simulation time. These figures show the contours for different concentrations in microgrammes per cubic metre under stable, neutral and unstable conditions. For comparison we have shown the concentrations obtained for a Gaussian plume in Figs. 6, 7 and 8 for stable, neutral and unstable conditions.

Stable conditions are the worst for trapping pollution. If we compare Figs. 3 and 6, we can see that pronounced effect of advection, which is not brought out by the Gaussian plume. Thus, the Gaussian plume would indicate a concentration below $200 \mu\text{g}/\text{m}^3$ at all points beyond, 16 km downstream, but if advection is considered, the concentrations after 5 hours would fall below $200 \mu\text{g}/\text{m}^3$ only beyond 30 km downstream from the stack. But, at larger distance, say at 40 km, the difference is negligible at the ground surface,

Similarly, if we compare Figs. 4 with 7 and 5 with 8 we can see much more effect of advection, which is not brought out by the Gaussian plume.

Acknowledgements

I am extremely thankful to Dr. P.K. Das, Director General of Meteorology for his guidance and his helpful suggestions from time to time without which this work would not have been possible to carry out. Thanks are also due to Dr. B. Padmanabhamurty, who has given me necessary facilities to carry out this job.

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Appendix 1

Determination of Stability

In the present model variation of wind speed and eddy diffusivities in the vertical has been considered which depends on the turbulence types or stability class. Similarly, plume rise for the buoyant plumes and the horizontal and vertical diffusion coefficients (*i.e.*, standard deviation of pollutants distribution) also vary according to the stability classes. Therefore, it is necessary to determine the stability of the atmosphere within the planetary boundary layer. The determination of stability categories which are attributed to Pasquill 1962 has been made more objective by Turner (1964) by specifying the classes according to a net radiation index (NR) and wind speed, for the night time NR depends on cloudiness, for day time NR depends on solar altitude and cloudiness (Holzworth 1974).

Pasquill stability categories* as a function of net radiation index and wind speed, 1 Knot=0.515 m/s (after Turner 1964)

Wind speed (Knots)	Net radiation index (NR)						
	4	3	2	1	0	-1	-2
0, 1	1	1	2	3	4	6	7
2, 3	1	2	2	3	4	6	7
4, 5	1	2	3	4	4	5	6
6	2	2	3	4	4	5	6
7	2	2	3	4	4	4	5
8, 9	2	3	3	4	4	4	5
10	3	3	4	4	4	4	5
11	3	3	4	4	4	4	4
12	3	4	4	4	4	4	4

*The stability categories 1, 2, ..., 6 correspond to A, B, ..., F and seventh class, extremely stable, G, has been added.

Insolation as a function of solar altitude
(After Turner 1964)

Solar altitude (a)	Insolation	Insola- tion class number (IN)
$60^\circ < a$	Strong	4
$35^\circ < a \leq 60^\circ$	Moderate	3
$15^\circ < a \leq 35^\circ$	Slight	2
$a \leq 15^\circ$	Weak	1

In the present computerized model, the stability classes has been determined according to

cloudiness, wind and solar altitude corresponding to the latitude of station culled out of *Smithsonian Meteorological Tables* (List 1957).