

Two-dimensional analytical model for estimating crosswind integrated concentration in a capping inversion: eddy diffusivity as a function of downwind distance from the source

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Abstract

A mathematical model has been proposed for computing crosswind-integrated concentration in a capping inversion layer by considering the eddy diffusivity as a function of down wind distance from the source. An analytical solution of the resulting partial differential equation with the physically relevant boundary conditions has been obtained for the general functional form of eddy diffusivity using the method of eigen-function expansion.

The model with eddy diffusivity as a linear function of downwind distance is validated with the available data in the literature from Copenhagen in Denmark and plume validation experiment conducted by Electric Power Research Institute at Kincaid in USA. The agreement is found to be good between the computed and the observed concentrations in both the experiments. In fact, majority of the concentrations predicted from the model are within a factor of two to observations.

Keywords: Mathematical model; Dispersion; Crosswind-integrated concentration; Eddy diffusivity; Eigen-function expansion

1. Introduction

Atmospheric dispersion models are needed for impact assessment, siting of industrial and residential complexes, emergency preparedness, planning and management, and related matters. A dispersion model plays a crucial role as a part of methodology to develop air quality criteria. The factors largely responsible for the dispersion include the physical and chemical nature of emissions, prevailing meteorological conditions, location of the source and terrain characteristics. Dispersion of pollutants in the atmosphere is governed by the following dominant mechanisms (Wark and Warner, 1981): (i) mean air-flow that transports the pollutants

down wind and (ii) turbulent velocity fluctuations that disperse the pollutants in all directions. It is required to parameterize turbulence and the wind velocity in the formulation of atmospheric dispersion models.

Analytical models are extensively used for the air quality analysis by the enforcement agencies. Gaussian models are widely used (Seinfeld, 1986; Zammetti, 1990) for this purpose and they have their own limitations. Assuming eddy diffusivities and the wind velocity to be constant, the governing equations in the Gaussian models are solved analytically (Hanna et al., 1982). For the practical applications of the solution obtained, eddy diffusivities are expressed as functions of down wind distance through dispersion parameters and the wind speed is parameterized as the power law function of height above the ground (Irwin, 1979). This approach is widely accepted from application point of view, however, mathematically it is inconsistent (Llewelyn,

1983; Sharan et al., 1996a, b). Nieuwstadt (1980) has used a quadratic polynomial, vanishing at the ground and top of the finite mixed layer, for vertical eddy diffusivity in the development of an air quality model. Recently, Otte and Wyngaard (1996) have extended the same concept to the planetary boundary layer modeling. Analytical models have been developed (Yeh and Haung, 1975; Lin and Hildemann, 1996, 1997) for the atmospheric-dispersion in both bounded (inversion) and unbounded (infinite mixing layer) domains by expressing both eddy diffusivities and wind speed as a power law functions of height. Tirabassi and his coworkers (Lupini and Tirabassi, 1979, 1983; Tirabassi, 1989) have also used height dependent wind speed as well as eddy diffusivities to obtain solutions of advection-diffusion equation.

Recently, it has been emphasized (Arya, 1995; Sharan et al., 1996a; Sharan and Yadav, 1998) that for the treatment of near source dispersion, eddy diffusivities are parameterized as a linear function of down wind distance from the source. This has been used in dispersion models in convective (Sharan et al., 1996a) and stable (Sharan and Yadav, 1998) weak wind conditions.

It is recognized that the planetary boundary layer (PBL) is often capped by an inversion, which simply reflects back the material reaching the inversion base (Arya, 1999). The earlier models (Sharan et al., 1996a, b; Sharan and Yadav, 1998) imply unrestricted diffusion of plume in the vertical direction. This does not happen in the real atmosphere where a finite layer of vanishing turbulence at the top of the PBL restricts vertical diffusion within the PBL.

In the present study, we formulate a model for dispersion of pollutants released from an elevated source in a surface-based inversion layer for crosswind-integrated concentration by considering the eddy diffusivities as a function of down wind distance from the source. A closed form solution of the resulting partial differential equation is obtained for the arbitrary functional form of eddy diffusivity using the method of eigen-function expansion.

2. Mathematical description

The steady state concentration (c) of a pollutant in the atmosphere is governed by the advection-diffusion equation (Seinfeld, 1986):

$$U \frac{\partial c}{\partial x} = \frac{\partial}{\partial x} \left(K_x \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial c}{\partial z} \right), \quad (1)$$

where U is the uniform wind speed K_x , K_y and K_z are, respectively, the eddy diffusion coefficients along x , y and z directions. x -axis is oriented in the direction of the mean wind.

The crosswind average concentration is obtained by integrating Eq. (1) with respect to y from $-\infty$ to ∞ .

$$U \frac{\partial \bar{c}}{\partial x} = \frac{\partial}{\partial x} \left(K_x \frac{\partial \bar{c}}{\partial x} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial \bar{c}}{\partial z} \right). \quad (2)$$

Under moderate to strong winds, the transport due to advection dominates over that due to longitudinal diffusion:

$$\left| U \frac{\partial \bar{c}}{\partial x} \right| \gg \left| \frac{\partial}{\partial x} \left(K_x \frac{\partial \bar{c}}{\partial x} \right) \right| \quad (3)$$

and thus, we neglect the longitudinal diffusion term. Eq. (2) becomes

$$U \frac{\partial \bar{c}}{\partial x} = \frac{\partial}{\partial z} \left(K_z \frac{\partial \bar{c}}{\partial z} \right). \quad (4)$$

This is subject to the following boundary conditions:

(i) The no-flux condition at the ground:

$$z = 0, \quad \frac{\partial \bar{c}}{\partial z} = 0. \quad (5a)$$

(ii) The pollutant can not penetrate through the layer located at a height H and accordingly,

$$\text{at } z = H, \quad \frac{\partial \bar{c}}{\partial z} = 0, \quad (5b)$$

where H is the height of the inversion layer above the ground.

(iii) The pollutant is released from an elevated source of strength Q located at $(0, h_s)$ and we have

$$\text{at } x = 0, \quad U \bar{c}(0, z) = Q \delta(z - h_s); \quad 0 \leq h_s < H, \quad (5c)$$

where h_s is the stack height and δ is the Dirac delta function. The Dirac delta function $\delta(z - h_s)$ vanishes everywhere except at the point $z = h_s$ and it has unit area under the curve in the interval containing $z = h_s$, i.e.,

$$\int_{-\infty}^{\infty} \delta(z - h_s) dz = 1.$$

The Gaussian model is essentially based on Fickian diffusion theory and the solution is obtained by assuming constant apparent eddy diffusivity K_z , which is parameterized in the solution in terms of dispersion parameter σ representing the growth of the plume as a function of downwind distance. For the case of onshore flow over a coastline, where inland areas are progressively unstable, one can expect the eddy diffusivity as a function of downwind distance. Here we take the eddy diffusivity K_z as a function of distance downwind from the source (Arya, 1995), i.e.,

$$K_z = K(x). \quad (6)$$

Since the pollutant particles travel downwind at a constant speed, this is equivalent to assuming that the diffusion coefficient in the vertical direction is a function of the downwind flight time (Ermak, 1977). An analogous situation occurs in the theory of Brownian

motion where the diffusion coefficient of the Brownian particles is a function of time (Chandrasekhar, 1943).

Using (6), Eq. (4) reduces to:

$$U \frac{\partial \bar{c}}{\partial x} = K(x) \frac{\partial^2 \bar{c}}{\partial z^2}. \quad (7)$$

The resulting parabolic partial differential Eq. (7) (describing cross-wind integrated concentration) with eddy diffusivity as a function of downwind distance can be solved, in principle, numerically. One of the boundary condition is prescribed in terms of Dirac delta function representing a point source. The various approaches are used to approximate Dirac delta function for describing a point source in the numerical models. Some of them used the Gaussian distribution function. Kansa and Carlson (1992) have used a function of the form

$$\delta(x - 1/2) = 120/(1 + v^2) \text{ in which } v = 120(x - 1/2),$$

to represent the Dirac delta function around the point $x = 1/2$. Third approach has been to distribute the mass uniformly at a number of grid points located in the neighborhood of a point source. Recently, Kansa (personal communication) has pointed out to approximate the Dirac delta function in terms of a triangular function. However, the representation/resolution of a point source in the numerical dispersion models is an open problem in the literature. An alternative approach avoiding this problem is based on the Lagrangian Particle dispersion modeling (Sharan and Gopalakrishnan, 2002).

In the present study, we solve Eq. (7) for arbitrary functional form of K with x analytically to obtain a closed form solution.

2.1. Solution

Eq. (7) represents a parabolic partial differential equation with variable coefficients. Both the boundary conditions (5a and 5b) with respect to z are homogeneous. Eq. (7) with the boundary conditions 5(a)–(c) can be treated as an eigenvalue problem (Zauderer, 1983). The problem of determining a nonzero solution of a homogeneous differential equation with homogeneous boundary conditions is known as an eigenvalue problem.

A solution to Eq. (7) satisfying the boundary conditions (5a and 5b) is given by (Appendix A):

$$\begin{aligned} \bar{c}(x, z) = & A_0 + \sum_{n=1}^{\infty} A_n \cos(\beta_n z) \\ & \times \exp\left\{-\frac{\beta_n^2}{U} \int_0^x K(x') dx'\right\}, \end{aligned} \quad (8)$$

where $\beta_n = n\pi/H$ and A_i , $i = 0, 1, 2, \dots$ is the set of infinite coefficients which need to be determined using condition (5c).

2.2. Estimation of coefficients

Condition (5c) using (8) can be written as

$$A_0 + \sum_{n=1}^{\infty} A_n \cos(\beta_n z) = \frac{Q}{U} \delta(z - h_s). \quad (9)$$

Notice that 0 and β_n ($n \geq 1$) are the eigenvalues of the operator $-d^2/dz^2$. The corresponding eigenvectors are:

$$1, \cos(\beta_n z), n \geq 1. \quad (10)$$

We will use the orthogonal property of the eigenvectors. Multiplying Eq. (9) by the eigenvectors $1, \cos(\beta_n z)$; $n \geq 1$ and integrating with respect to z from 0 to H , we find

$$\begin{aligned} A_0 &= \frac{Q}{HU}, \\ A_n &= \frac{2Q}{HU} \cos(\beta_n h_s), \quad n \geq 1. \end{aligned} \quad (11)$$

Finally, the solution of (7) is given by

$$\begin{aligned} \bar{c}(x, z) = & \frac{Q}{HU} \left[1 + 2 \sum_{n=1}^{\infty} \cos(\beta_n h_s) \cos(\beta_n z) \right. \\ & \left. \times \exp\left\{-\frac{\beta_n^2}{U} \int_0^x K(x') dx'\right\} \right]. \end{aligned} \quad (12)$$

Eq. (12) provides the crosswind average concentration of a pollutant, released from an elevated point source, in the atmosphere with eddy diffusivity depending on the down wind distance from the source. Eq. (12) can be expressed as (Whittaker and Watson, 1958)

$$\begin{aligned} \bar{c}(x, z) = & \frac{Q}{2\sqrt{\pi U f(x)}} \left\{ \sum_{n=-\infty}^{\infty} \left[\exp\left\{-\frac{U}{4f(x)}(z + h_s - 2nH)^2\right\} \right. \right. \\ & \left. \left. + \exp\left\{-\frac{U}{4f(x)}(z - h_s - 2nH)^2\right\} \right] \right\}, \end{aligned} \quad (13)$$

where

$$f(x) = \int_0^x K(x') dx'. \quad (14)$$

Eq. (13) may be interpreted as the contribution from a source term located at $z = h_s$ and its successive images by reflection from two parallel boundaries at $z = 0$ and $z = H$, respectively (Hanna et al., 1982; Seinfeld, 1986). The exponential terms in the summation in (13) converge rapidly even close to the source.

Notice that in the limit $H \rightarrow \infty$ only the term corresponding to $n = 0$ contributes to the summation in Eq. (13) and one obtains

$$\begin{aligned} \bar{c}(x, z) = & \frac{Q}{2\sqrt{\pi U f(x)}} \left\{ \exp\left\{-\frac{U}{4f(x)}(z + h_s)^2\right\} \right. \\ & \left. + \exp\left\{-\frac{U}{4f(x)}(z - h_s)^2\right\} \right\}. \end{aligned} \quad (15)$$

Physically, $H \rightarrow \infty$ indicates the absence of inversion lid (Hanna et al., 1982).

From the application point of view, one is interested in the pollutant concentration at the ground. The concentration at the ground is obtained by putting $z = 0$ in Eq. (12) and it is given by

$$\bar{c}(x, 0) = \frac{Q}{HU} \left[1 + 2 \sum_{n=1}^{\infty} \cos(\beta_n h_s) \times \exp \left\{ -\frac{\beta_n^2}{U} \int_0^x K(x') dx' \right\} \right]. \quad (16)$$

The ground level concentration is influenced with the functional form of the eddy diffusivity.

2.3. Ground level source

Putting $h_s = 0$ in Eq. (13) to obtain concentration distribution for a ground level source.

$$\bar{c}(x, z) = \frac{Q}{\sqrt{\pi U f(x)}} \sum_{n=-\infty}^{\infty} \exp \left\{ -\frac{U}{4f(x)} (z - 2nH)^2 \right\}. \quad (17)$$

For practical applications, expression (17) can be used for computing the concentration distribution of the pollutants released from a line source.

Solution (13) gives the crosswind-integrated concentration from an elevated release in a finite layer when the eddy diffusivity is a function of down wind distance from the source. The corresponding relation for a ground level release is given by Eq. (17). In the absence of the inversion layer, the relation for the crosswind-integrated concentration is obtained by taking the limit as $H \rightarrow \infty$ in Eq. (13).

2.4. Particular cases

1. Eddy diffusivity is taken as a constant K_0 , we get from (13):

$$\bar{c}(x, z) = \frac{Q}{2\sqrt{\pi U K_0 x}} \left\{ \sum_{n=-\infty}^{\infty} \left[\exp \left\{ -\frac{U}{4K_0 x} (z + h_s - 2nH)^2 \right\} + \exp \left\{ -\frac{U}{4K_0 x} (z - h_s - 2nH)^2 \right\} \right] \right\}. \quad (18)$$

Expressing (18) in terms of dispersion parameters using the relation $\sigma^2 = 2K_0 x/U$, we get

$$\bar{c}(x, z) = \frac{Q}{\sqrt{2\pi U \sigma}} \sum_{n=-\infty}^{\infty} \left[\exp \left\{ (z + h_s - 2nH)^2 / 2\sigma^2 \right\} + \exp \left\{ -(z - h_s - 2nH)^2 / 2\sigma^2 \right\} \right], \quad (19)$$

which is the well-known Gaussian model for an elevated source with multiple reflections from two parallel boundaries at $z = 0$ and H .

2. Eddy diffusivity: as a linear function of down wind distance:

Eddy diffusivity $K(x)$ can be parameterized as a linear function of down wind distance (Arya, 1995; Sharan et al., 1996a; Sharan and Yadav, 1998):

$$K(x) = \alpha \bar{U}_A x, \quad (20)$$

where x is the distance along the mean wind from the source, \bar{U}_A is the average wind speed obtained by taking the average of the wind in the layer bounded by two parallel lines $z = 0$ and $z = H$. The parameter α is identified as the turbulence intensity (Arya, 1995).

Using (20), Eq. (12) becomes

$$\bar{c}(x, z) = \frac{Q}{HU} \left[1 + 2 \sum_{n=1}^{\infty} \cos(\beta_n h_s) \cos(\beta_n z) \times \exp \left(-\frac{\beta_n^2 \alpha \bar{U}_A x^2}{2U} \right) \right]. \quad (21)$$

3. Results and discussion

The crosswind integrated concentrations are estimated from Eq. (21) at $z = 0$. The turbulence parameter α is parameterized as

$$\alpha = \left(\frac{\sigma_w}{U} \right)^2, \quad (22)$$

where σ_w is the standard deviation of the vertical component of the velocity. For computing the concentration using Eq. (21), we require the source strength Q , effective stack height h_s , inversion height H , the wind velocity in the layer and the σ_w from the turbulence measurements. In the absence of turbulence measurements, σ_w can be parameterized in terms of convective velocity scale W_* in unstable conditions and frictional velocity u_* in stable conditions (Sharan et al., 1996a and Sharan and Yadav, 1998). W_* and u_* can be estimated from the similarity theory using tower observations.

The corresponding concentration from the Gaussian model is obtained from Eq. (19). The dispersion parameter σ in (19) is taken from the Briggs's formulations (Briggs, 1975). We propose to validate the model with the available data in the literature from Copenhagen in Denmark (Gryning et al., 1987) and EPRI experiment (Hanna and Paine, 1987).

Atmospheric dispersion experiments were carried out (Gryning and Lyck, 1984; Gryning et al., 1987) in the northern part of Copenhagen under neutral and unstable conditions. The tracer SF_6 was released from a tower at a height of 115 m. The site was mainly residential with a roughness length of ~ 0.6 m. The parameters such as inversion height (H), wind speed (U) and σ_w reported in Table 1 are taken from Gryning et al. (1987). The observed values for the crosswind-integrated

Table 1

Observed and computed crosswind-integrated concentrations (C/Q) at ground in diffusion experiments in northern part of Copenhagen (Gryning et al., 1987) with $h_s = 115\text{m}^a$

Run No.	Date	PG stability	H (m)	U (m s^{-1})	σ_w (m s^{-1})	Distance from source (m)	$C/Q(10^{-4}\text{ s m}^{-2})$		
							Observed	Computed present model	Computed Gaussian model
1	20-09-78	A	1980	3.4	0.83	1900	6.48	4.91	4.59
1	20-09-78	A	1980	3.4	0.83	3700	2.31	2.58	2.24
2	26-09-78	C	1920	10.6	1.07	2100	5.38	3.06	1.73
2	26-09-78	C	1920	10.6	1.07	4200	2.95	1.71	0.89
3	19-10-78	B	1120	5.0	0.68	1900	8.20	5.59	3.12
3	19-10-78	B	1120	5.0	0.68	3700	6.22	3.09	1.53
3	19-10-78	B	1120	5.0	0.68	5400	4.30	2.15	0.99
4	3-11-78	C	390	4.6	0.47	4000	11.66	4.08	2.15
5	9-11-78	C	820	6.7	0.71	2100	6.72	4.68	2.73
5	9-11-78	C	820	6.7	0.71	4200	5.84	2.59	1.40
5	9-11-78	C	820	6.7	0.71	6100	4.97	1.81	0.97
6	30-04-78	C	1300	13.2	1.33	2000	3.96	2.55	1.45
6	30-04-78	C	1300	13.2	1.33	4200	2.22	1.38	0.71
6	30-04-78	C	1300	13.2	1.33	5900	1.83	1.00	0.51
7	27-06-78	B	1850	7.6	0.87	2000	6.70	4.04	1.95
7	27-06-78	B	1850	7.6	0.87	4100	3.25	2.17	0.89
7	27-06-78	B	1850	7.6	0.87	5300	2.23	1.70	0.67
8	06-07-78	D	810	9.4	0.72	1900	4.16	4.27	3.45
8	06-07-78	D	810	9.4	0.72	3600	2.02	2.82	2.30
8	06-07-78	D	810	9.4	0.72	5300	1.52	2.01	1.78
9	19-07-78	C	2090	10.5	0.98	2100	4.58	3.26	1.74
9	19-07-78	C	2090	10.5	0.98	4200	3.11	1.86	0.90
9	19-07-78	C	2090	10.5	0.98	6000	2.59	1.33	0.63

^aRMSE (with present model) = $2.38 \times 10^{-4}\text{ s m}^{-2}$, RMSE (with Gaussian model) = $3.49 \times 10^{-4}\text{ s m}^{-2}$.

concentrations are also taken from Gryning et al. (1987). The stability classification is chosen on the basis of the values of Monin–Obukhov length L . As the site was primarily residential, dispersion parameters for urban terrain are considered in the computation of concentration in the Gaussian model. The concentrations estimated from the present as well as the Gaussian models are also given in Table 1. This shows that the concentrations predicted from the model are in good agreement with those observed. Most of the concentrations are predicted with in a factor of 2. The concentrations computed from the present model are closure to the observations than those obtained from Gaussian model. The root mean square error (RMSE) is calculated from the formula:

$$\text{RMSE} = \sqrt{\sum_{i=1}^N (C_i^c - C_i^o)^2 / N}, \quad (23)$$

where C^c and C^o denote the calculated and observed concentrations and N is the number of measurements. The root mean square errors for the present model and the Gaussian model are 2.38×10^{-4} and

$3.49 \times 10^{-4}\text{ s m}^{-2}$, respectively. In the computation of RMSE, the concentration is referred to Q . Since the measurement site was mainly residential with a roughness length of about 0.6 m, we have considered the terrain as urban to calculate the dispersion parameter in the Gaussian model. However, the root mean square error is found to reduce from 3.49 to 1.82 by considering the site as rural.

The Electric Power Research Institute (EPRI) conducted a plume validation field experiment (Hudischewskyj and Reynolds, 1983) in 1980 and 81 at Kincaid (a flat site near Springfield, Illinois, USA). During the experiment, extensive meteorological observations were taken together with the stack characteristics and tracer data (Myers and Reynolds, 1984). Hourly ground level concentrations due to SF_6 from a 187 m stack were observed by a network of about 200 monitors, spread on arcs at downwind distances ranging from 0.5 to 50 km during convective conditions. For the model validation, we have chosen the same data as taken by Hanna and Paine (1987). The values of Q , U , H , W^* (convective velocity scale) given in Table 2 are

Table 2

Dispersion conditions of diffusion tests in EPRI experiment at Kincaid (Bowne et al., 1983; Hanna and Paine, 1987) with $h_s = 187$ m^a

Run No.	Date	Hr	PG stability	Q (g s ⁻¹)	H (m)	U (m s ⁻¹)	W_* (m s ⁻¹)	σ_w (m s ⁻¹)
1	25-4-80	12	A	11.2	893	2.3	0.76	1.79
2	25-4-80	13	A	11.2	1032	2.3	0.75	1.79
3	25-4-80	14	A	11.3	1175	3.3	0.89	1.86
4	25-4-80	15	B	11.1	1355	2.4	0.74	1.01
5	25-4-80	16	C	11.3	1539	3.4	0.93	1.83
6	25-4-80	17	C	10.7	1545	2.8	0.73	1.33
7	4-5-80	10	B	11.2	850	2.8	0.58	1.86
8	4-5-80	11	A	11.2	1447	2.8	0.62	2.33
9	4-5-80	12	A	11.2	1911	2.5	0.69	2.60
9	4-5-80	12	A	11.2	1911	2.5	0.73	2.60
10	7-5-80	10	B	16.2	950	4.0	0.83	1.84
11	7-5-80	11	B	12.0	1253	4.5	0.57	2.09
12	7-5-80	12	B	11.1	1548	5.1	0.80	2.28
13	9-5-80	11	A	12.1	1700	3.1	0.80	2.48
14	9-5-80	12	A	12.0	1750	2.1	0.41	2.58
15	13-7-80	10	B	10.2	226	3.3	0.40	1.15
16	13-7-80	11	A	12.3	241	2.9	0.41	1.32
17	13-7-80	12	A	14.5	275	2.0	0.41	1.49
18	13-7-80	13	A	14.6	396	1.9	0.45	1.59
19	13-7-80	14	B	13.2	554	2.0	0.45	1.83
20	13-7-80	15	B	13.2	600	1.7	0.59	1.77
21	13-7-80	16	B	13.5	600	1.6	0.46	1.66
22	13-7-80	17	B	14.3	600	1.9	0.39	1.34
23	13-7-80	18	C	14.9	619	2.7	0.33	1.12
24	20-7-80	9	C	18.3	121	7.7	0.46	0.98
26	24-7-80	15	B	13.7	1750	1.9	0.74	2.64
27	24-7-80	16	B	13.9	1750	1.9	0.64	2.36
28	16-5-81	10	C	16.4	856	6.2	0.53	1.85
29	16-5-81	11	C	16.7	1014	6.8	0.62	1.98
30	17-5-81	10	C	17.9	217	6.4	0.45	0.84
31	17-5-81	11	C	17.4	251	5.5	0.36	0.64
33	24-5-81	16	C	17.1	485	5.5	0.29	0.86
34	24-5-81	17	C	17.5	497	4.6	0.25	0.99
35	24-5-81	18	C	18.3	1002	5.2	0.21	0.90
36	28-5-81	11	A	12.2	823	2.7	0.58	2.02
37	28-5-81	12	A	13.0	1124	2.6	0.77	2.13
38	28-5-81	13	A	13.2	1250	3.2	0.82	2.21
39	28-5-81	18	D	12.7	1851	4.3	0.80	1.37
40	1-6-81	7	D	16.5	856	7.7	0.22	0.52

^aWind speed, U is observed at a height of 187 m.

taken from Hanna and Paine (1987). The values for σ_w are taken from the measurements taken from acoustic sounder. The PG stability is taken from the data reported in EPRI database.

The plume rise is calculated using the formulation for a buoyant plume from Briggs (1969). The fraction of the plume that penetrates the elevated layer is taken into account (Weil and Brower, 1984) in the computation of plume rise. The modification of the effective stack height for plumes trapped within the mixed layer is based on the assumption that the plume rise due to penetration is linearly varying between $0.62 H$ for no penetration to H

for full penetration. The values of the parameters required for the plume rise calculation are taken from the measurements (Myers and Reynolds, 1984).

The observed crosswind integrated concentrations are taken from Hanna and Paine (1987). The corresponding concentrations are computed from the present model and the Gaussian model up to a down wind distance of 10 km. In the Gaussian plume model, dispersion parameters estimated from Briggs analytical expressions for rural terrain (Zannetti, 1990) are used.

Fig. 1 gives the scatter diagram of the ratio of the model-predicted to observed concentration versus the

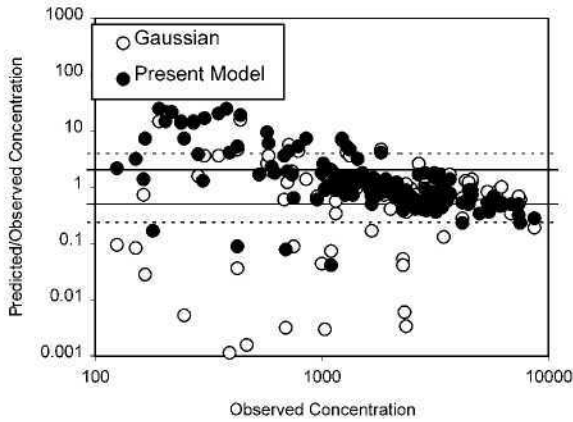


Fig. 1. Ratio of predicted and observed concentrations with observed concentration for the present and Gaussian models.

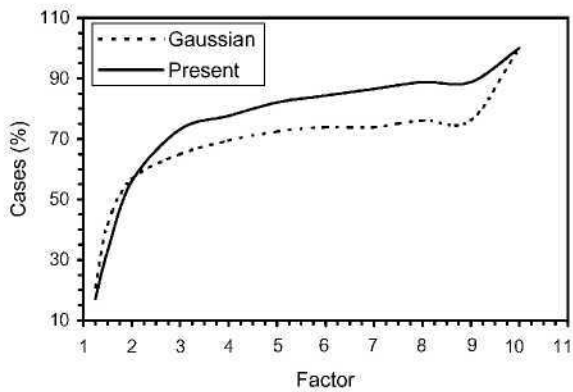


Fig. 2. Percentage of cases predicted with in a given factor using the present model and the Gaussian model.

observed concentration for the current and Gaussian models. The points lying in-between the two solid lines are predicted with in a factor of two. The dashed lines in the figure indicate a factor of four. Fig. 2 provides a more objective picture regarding the model predictions. It shows that about 56% of the predicted cases are with in a factor of 2 and more than 82% with in a factor of 5. The figure also reveals that the performance of the present model is comparable with that of Gaussian model in terms of the percentage of cases predicted up to a factor of two. The percentage of cases predicted by the present model is higher than those with the Gaussian model with in a factor larger than two.

Other way of evaluating the performance of the model is through quantile-quantile ($Q-Q$) comparisons of predicted and observed concentration distributions (Olesen, 1995; Venkatram, 1999; Venkatram et al., 2001). Venkatram (1999) has discussed the usefulness of $Q-Q$ analysis. We create the $Q-Q$ plot by first ranking

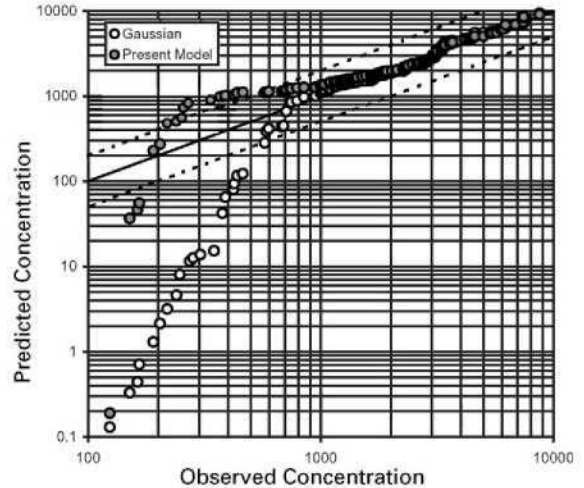


Fig. 3. $Q-Q$ plot between the observed and predicted concentrations in $\mu\text{g m}^{-2}$ for the present and Gaussian models. Middle line is the one-to-one line and the outer lines are the lines with factor two.

both the observations and model predictions from highest to lowest and then plotting the ranked observations versus ranked predictions using their magnitudes.

Fig. 3 shows a $Q-Q$ plot for both the present and Gaussian models. Both curves are close to the 1-1 line for the observed concentrations $> 800 \mu\text{g m}^{-2}$. The curve for the Gaussian model falls off quickly below the one-to-one line for observed concentrations $< 700 \mu\text{g m}^{-2}$ and a major fraction of the predicted concentrations fall below the factor-of-two line. In this case, the concentrations predicted from the present model are relatively closer to the one-to-one line than those computed from the Gaussian model.

4. Conclusions

A mathematical model is formulated by parameterizing the eddy diffusivity as a function of down wind distance from the source for computing the crosswind-integrated concentration in a finite layer released from an elevated/ground-level source. A closed-form solution for the resulting partial differential equation with general functional form of eddy diffusivity is determined using the method of eigen-function expansion. The various particular cases are deduced.

The model with a linear function for eddy diffusivity is validated with the available data in the literature from Copenhagen in Denmark (Gryning et al., 1987) and EPRI experiment at Kincaid in USA (Hanna and Paine, 1987). The agreement is found to be good between the computed and the observed concentrations in both the experiments. In fact, majority of the concentrations

predicted from the model are within a factor of two to observations. In the Copenhagen experiment, the value of RMSE from the present model ($2.38 \times 10^{-4} \text{ s m}^{-2}$) is found to be smaller than that from the Gaussian model ($3.49 \times 10^{-4} \text{ s m}^{-2}$). In the EPRI experiment, 82% of the total cases are predicted within a factor of five from the present model where it was about 72% in the case of Gaussian model. The overall performance of the present model is found to be better than the Gaussian model and this may be because of the fact that on-site turbulent observations have been used to estimate the turbulent intensity. In both the cases, the data used for the purpose of validation is under convective conditions. However, the observations for the crosswind-integrated concentrations in stable conditions are very limited and the model needs to be validated with the availability of data in a stable atmosphere. In the present study, an alternative approach has been proposed for computing the crosswind-integrated concentration. This approach takes care for some of the inherent limitations of the Gaussian model. The proposed model can also be used for computing the concentration distribution from a line source.

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Appendix A

We take the solution of Eq. (7) of the form

$$\bar{\alpha}(x, z) = \sum_n X_n(x) Z_n(z). \quad (\text{A.1})$$

Differentiating (A.1) partially with respect to x and z and substituting in Eq. (7), then we obtain the ordinary differential equations in x and z as for each n ,

$$\frac{d^2 Z_n}{dz^2} = -\beta_n^2 \quad (\text{A.2})$$

and

$$\frac{dX_n}{dx} = -\frac{K(x)}{U} \beta_n^2, \quad (\text{A.3})$$

where β_n^2 is a constant.

The general solution of Eq. (A.2) is given by:

$$Z_n(z) = B'_n \sin(\beta_n z) + A'_n \cos(\beta_n z), \quad (\text{A.4})$$

where A'_n and B'_n are constants.

Using the boundary conditions obtained from Eq. 5(a), 5(b) and (A.1) in Eq. (A.4), we find

$$B'_n = 0 \quad \text{for } n \geq 1 \quad (\text{A.5})$$

and

$$\beta_n = \frac{n\pi}{H} \quad \text{for } n \geq 1. \quad (\text{A.6})$$

For $n = 0$, $\beta_0 = 0$, the solution of (A.2) with corresponding boundary conditions is a constant, i.e.,

$$Z_0(z) = A'_0. \quad (\text{A.7})$$

The general solution of Eq. (A.3) is given by

$$X_n(x) = d_n \exp\left\{-\frac{\beta_n^2}{U} \int_0^x K(x') dx'\right\}, \quad (\text{A.8})$$

where d_n are constants.

Using relations (A.4), (A.7) and (A.8), solution (A.1) can be written as

$$\bar{\alpha}(x, z) = A_0 + \sum_{n=1}^{\infty} A_n \cos(\beta_n z) \times \exp\left\{-\frac{\beta_n^2}{U} \int_0^x K(x') dx'\right\}, \quad (\text{A.9})$$

where A_i , $i = 0, 1, 2, \dots$ is the set of infinite coefficients.

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