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RESEARCH ARTICLE

Simulation Herimitized Atmospheric Concentration Using different Intensity Parameters

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Abstract

Solutions of three dimensional herimitized advection diffusion equation of air pollutant from a point source at a vertical height with eddy diffusivities which are depending on downwind distance, turbulent parameters and segmented plume, are compared with observed Copenhagen concentrations data.

Introduction

The vertical diffusion of a passive tracer release from a point source in unstable and stable atmosphere has been studied by an analytical solution of the advection-diffusion equation.

On the other hand predicted ground level concentration, regardless of the atmospheric boundary layer (ABL) scenario are underestimates the experimental data (Irwin 1983). In fact, although the ABL is assumed to have infinite height, its actual vertical limit affects the behavior of all quantities. Non-Gaussian approaches are proved to perform more reliably, despite the more complicated parameterization of the ABL dynamics (Hinrichson, 1986; Tirabassi et al., 1986; Brown et al., 1989; Van Ulden, 1992; Sharan et al., 1996; Lin and Hildemann, 1997). Turbulent intensities were observed to be as high as 44% for longitudinal component, 37% for lateral and 30% vertical component in weak wind stable condition (Agarwal et al. 1995).

Roberts (1923) has obtained the solution of the diffusion equation in downwind distance considering the eddy diffusivities to be constant.

Arya (1995) has been solved advection diffusion equation taking the eddy diffusivities as function in downwind distance.

Recently Essa et al. (2007) have obtained an analytical solution of the hermitized diffusion equation with eddy diffusivities varying linearly with downwind distance from the source and turbulence parameters. The computed results from the model are found under predicted with observations in the convective conditions. This model and Gaussian model using different shapes of eddy diffusivities are compared with observation concentrations which measured above Copenhagen, Denmark. Some statistical values are calculated.

Model formulation

Considering the self-adjoin diffusion equation in the steady state and the eddy diffusivities are functioned in downwind distance is given as follows (Essa et al .2007):

$$U\frac{\partial C}{\partial x}=\frac{\partial}{\partial x}(K_x\frac{\partial C}{\partial x})+\frac{\partial}{\partial y}(K_y\frac{\partial C}{\partial y})+\frac{\partial}{\partial z}(K_z\frac{\partial C}{\partial z})+0.5([\frac{\partial}{\partial x},u],-\sum_{i=x,y,z}[(\frac{\bar{\partial}}{\partial i}),\delta(i)K_i])C(x,y,z) \quad (1)$$

Where C is the mean concentration, K_x, K_y, and K_z are the eddy diffusivities in x, y and z respectively, $(\frac{\overleftarrow{\partial}}{\partial x})$) is the differential operator acts to the left and $\delta(x)$ is the Dirac delta function, U is taken to be constant and non-zero. The eddy diffusivities K are taken as linear function of downwind distance based on Taylor theory (1921) for small travel times (Arya, 1995) and Sharan (1996) in the form:

$K_x = \alpha U x$, $K_y = \beta U x$ and $K_x = \gamma U x$ (2)

Where α, β, and γ are turbulence parameters depending on atmospheric stability.

Substituting from equation (2) in equation (1) we get:

$$\alpha x\frac{\partial^2 C}{\partial x^2}+(\alpha-2)\frac{\partial C}{\partial x}+\frac{\bar{\delta}(x)C}{2}+\beta x\frac{\partial^2 C}{\partial y^2}+\gamma x\frac{\partial^2 C}{\partial z^2}-0.5([\frac{\bar{\partial}}{\partial y},\beta\delta(y)]+[\frac{\bar{\partial}}{\partial z},\gamma\delta(y)]C(x,y,z) \quad (3)$$

Equation (3) is considered under boundary conditions as follows:

(i) mass continuity of the source is located at the point (0,0,H)with strength Q using Dirac's delta function as follows:

$UC = Q\delta(y)\delta(z-H)$ at x=0 (4)

(ii) The concentration decrease to zero at far away from the source

$C \to 0$ at $x, y \, and \, z \to \infty$ (5)

(iii) Flux at the ground equal zero

$\frac{\partial C}{\partial z} = 0$ at $z = 0$ (6)

Equation (3) is solved under the above boundary conditions (4) to (6). The concentration formula for the ground source is given by (Essa et al. 2007) as follows:

$$C(x,y,z)=\frac{1}{U\pi\sqrt{\beta\gamma}x^2}[1+\frac{\alpha}{x^2}(\frac{y^2}{\beta}+\frac{z^2}{\gamma})]^{-(\frac{1}{\alpha}+1)} \quad (7)$$

If H ≠ 0 the solution becomes in the form:

$$\left.\begin{aligned}
C(x,y,z)&=\frac{1}{2U\pi\sqrt{\beta\gamma}x^2}[W_{z+H}+W_{z-H})]\\
W_{z+H}&=[1+\frac{\alpha}{x^2}(\frac{y^2}{\beta}+\frac{(z+H)^2}{\gamma})]^{-(\frac{1}{\alpha}+1)}\\
W_{z-H}&=[1+\frac{\alpha}{x^2}(\frac{y^2}{\beta}+\frac{(z-H)^2}{\gamma})]^{-(\frac{1}{\alpha}+1)}
\end{aligned}\right\} \quad (8)$$

Slender plume approximation:

One can get this approximation when the concentration close to the plume center line. Taking $\alpha \to 0$ in solution (8) we get Eq. (8) in the form:-

$$\left.\begin{aligned}
C(x,y,z)&=\frac{1}{2U\pi\sqrt{\beta\gamma}x^2}[(1+\alpha p)^{-(\frac{1}{\alpha}+1)}+(1+\alpha q)^{-(\frac{1}{\alpha}+1)})]\\
p&=\frac{1}{x^2}(\frac{y^2}{\beta}+\frac{(z+H)^2}{\gamma})\\
q&=\frac{1}{x^2}(\frac{y^2}{\beta}+\frac{(z-H)^2}{\gamma})]
\end{aligned}\right\}$$

Then $C = S_1 + S_2$

Where

$$S_1 = \frac{Q}{2U\pi\sqrt{\beta\gamma}x^2}(1+\alpha p)^{-(\frac{1}{\alpha}+1)}$$

$$S_2 = \frac{Q}{2U\pi\sqrt{\beta\gamma}x^2}(1+\alpha q)^{-(\frac{1}{\alpha}+1)}$$

Taking the limit $\alpha \to 0$ one gets $(1+\alpha p)^{\frac{-1}{\alpha p}} \to e$

$$S_1 = \frac{Q}{2\pi x\sqrt{\beta Ux}\sqrt{\gamma Ux}}\exp[-\frac{U}{x}(\frac{y^2}{\beta Ux}+\frac{(z+H)^2}{\gamma Ux})]$$

$$S_2 = \frac{Q}{2\pi x\sqrt{\beta Ux}\sqrt{\gamma Ux}}\exp[-\frac{U}{x}(\frac{y^2}{\beta Ux}+\frac{(z-H)^2}{\gamma Ux})]$$

Then

$$C(x,y,z) = \frac{Q}{2\pi x\sqrt{\beta Ux}\sqrt{\gamma Ux}}\exp(-\frac{y^2}{\beta x^2})\left[\exp-\left(\frac{(z+H)^2}{\gamma x^2}\right)+\exp-\left(\frac{(z-H)^2}{\gamma x^2}\right)\right] \quad (9)$$

If one replaces βx^2 by $2\sigma^2{}_y$ and γx^2 by $2\sigma^2{}_z$ one gets a form analogous to the Gaussian plume in the form

$$C(x,y,z) = \frac{Q}{2\pi U\sigma_y\sigma_z}\exp(-\frac{y^2}{2\sigma_y{}^2})[\exp-(\frac{(z+H)^2}{2\sigma_z{}^2})+\exp-(\frac{(z-H)^2}{2\sigma_z{}^2})] \quad (10)$$

Parameterization

One makes application of solution (8), taking the turbulence intensities in the form (Arya 1995)

$$\alpha = (\frac{\sigma_u}{U})^2,\ \beta = (\frac{\sigma_v}{U})^2,\ \gamma = (\frac{\sigma_w}{U})^2$$

Where σ_u , σ_v and σ_w are the standard deviations of wind speed in horizontal, lateral and vertical directions respectively. In the absent of direct measurements of σ_u , σ_v and σ_w , taking some relations in terms of wind speed U and friction velocity u_* as follows:

$$\alpha = 6.25(\frac{u_*}{U})^2,\ \beta = 3.6(\frac{u_*}{U})^2 \text{ and } \gamma = 1.69(\frac{u_*}{U})^2 \quad (11)$$

In this study, the tracer data are collected during unstable conditions (Gryning et al. (1987)) using equation (8) in terms of the parameterization for α , β , and γ in terms of $\frac{u_*}{U}$ (Eq. (11)). Also one can use the relations by Cirillo et al. (1992) in terms of standard deviation of wind direction σ_θ to calculate the turbulence parameters as follows:

$$\alpha = \cosh(\sigma_\theta{}^2)-1,\ \beta = \sinh(\sigma_\theta{}^2) \text{ and } \gamma = \frac{\sigma_z^2}{2x^2} \quad (12)$$

Where σ_θ is the standard deviation of horizontal wind direction and $\sigma_z = sx/((1+(x/a))^q)$, s,a and q are constants depend on atmospheric stability (Sharan et al. 1995) are shown in Table (1) as follows:

Table (1) The corresponding between s,a and q and the Pasquill classes

Pasquill classes	A	B	C	D	E	F
a (km)	0.927	0.370	0.283	0.707	1.07	1.17
s(m/km)	102	96.2	72.2	47.5	33.5	22.0
q	-1.918	-0.101	0.102	0.465	0.624	0.70

Table (2) methods are used to determine the concentrations

Methods for computed concentration (Bq/m^3)	Methods are used to determine the parameters α, β,and γ	The equations are using to determine the concentration
C1	$\frac{u_*}{U}$	Eq.(8), and Eq.(11)
C2	$\frac{u_*}{U}$	Eq.(9), and Eq.(11)
C3	σ_θ	Eq.(8), and Eq.(12)
C4	σ_θ	Eq.(9), and Eq.(12)
C5	σ_θ	Eq.(10), and Eq.(12)

Tracer Data

The performance of the C1, C2,…, C5 models have been evaluated against experimental ground-level concentration using tracer sulfur hexafluoride data from dispersion experiments carried out in the northern part of Copenhagen, Denmark described in Gryning et al. (1987).The tracer was released without buoyancy from a tower at a height of 115 m and was collected at the ground level positions at a maximum of three crosswind arcs of tracer sampling units. The sampling units were positioned of 2-6 km from the point of release. The tracer release typically started 1 h before the start of tracer sampling and stopped at the end of sampling period; the average sampling time was 1 h. The site was mainly residential with a roughness length of 0.6 m. Table 3 shows the meteorological data from Gryning and Lyck (1984) and Gryning et al. (1987) utilized during the experiments that were used for the validation of the proposed approach.

Table (3) Summary of meteorological conditions during the experiments

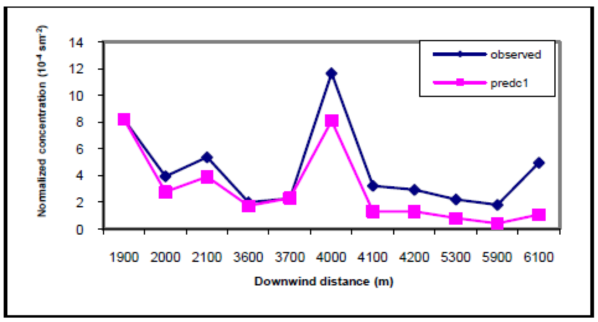
Exp.	*U(m /s)*	u_**(m/s)*	*L(m)*	σ_θ	z_i*(m)*
1	3.4	0.36	-37	0.20	1980
2	10.6	0.73	-292	0.50	1920
3	5.0	0.38	-71	0.36	1120
4	4.6	0.38	-133	0.99	390
5	6.7	0.45	-444	0.21	820
6	13.2	1.05	-432	0.58	1300
7	7.6	0.64	-104	0.67	1850
8	9.4	0.69	-56	0.42	810
9	10.5	0.75	-289	0.38	2090

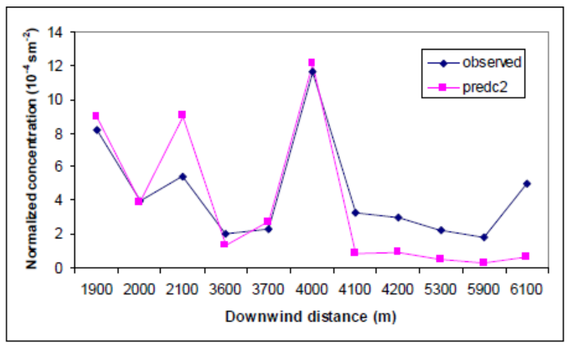
Table (4) Observed and modeled ground–level-cross-wind integrated concentrations $\overline{C}(x,0)/Q$ at different distance from the source.

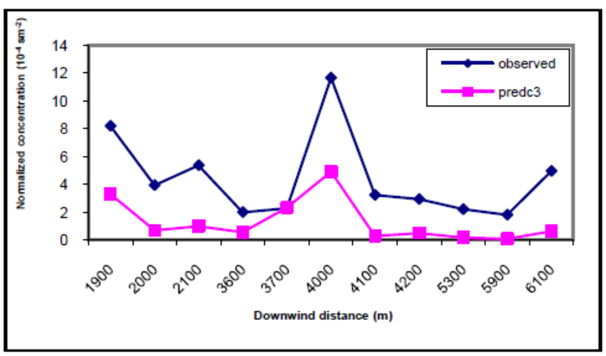
Exp.	Distance (m)	Observed (10^{-4} sm^{-2})	predictedc1 (10^{-4} sm^{-2})	predictedc2 (10^{-4} sm^{-2})	predictedc3 (10^{-4} sm^{-2})	predictedc4 (10^{-4} sm^{-2})	Predictedc5 (10^{-4} sm^{-2})
1	1900	6.48	7.48	8.45	7.62	7.62	7.62
	3700	2.31	2.33	2.70	2.35	2.35	2.35
2	2100	5.38	3.92	9.00	1.02	1.03	1.02
	4200	2.95	1.32	0.92	0.52	0.34	0.34
3	1900	8.2	8.20	8.91	3.31	3.32	3.31
	3700	6.22	4.93	2.10	1.17	1.18	1.17

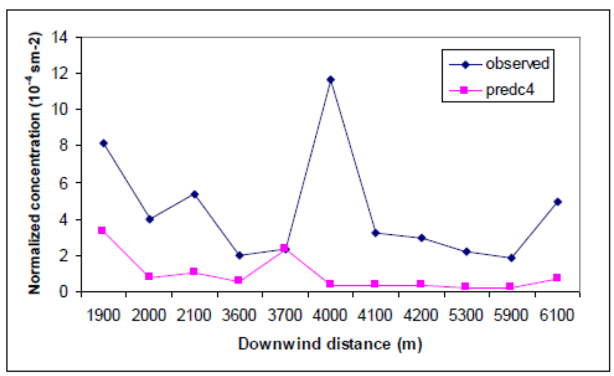
4	4000	11.66	8.11	12.16	4.92	0.35	9.67
5	2100	6.72	6.35	11.92	3.89	3.89	3.89
	4200	5.84	2.18	1.55	1.33	1.33	1.33
	6100	4.97	1.09	0.65	0.66	0.66	0.66
6	2000	3.96	2.79	3.88	0.71	0.73	0.71
	4200	2.22	0.81	0.52	0.21	0.21	0.21
	5900	1.83	0.43	0.25	0.11	0.20	0.11
7	2000	6.7	4.44	5.66	1.03	1.05	1.03
	4100	3.25	1.33	0.85	0.31	0.31	0.36
	5300	2.23	0.82	0.48	0.19	0.19	0.19
8	1900	4.16	4.60	6.13	1.53	1.54	1.53
	3600	2.02	1.75	1.29	0.58	0.58	0.56
	5300	1.52	0.86	0.52	0.32	0.28	0.55
9	2100	4.58	3.78	6.00	1.65	1.62	1.61
	4200	3.11	2.95	0.85	0.82	0.53	0.03
	6000	2.59	1.64	0.38	0.42	0.27	0.18

Table 4, shows the measured and computed ground- level concentrations through centerline released from high source *C (0, 0, H)* using five methods as explained before.









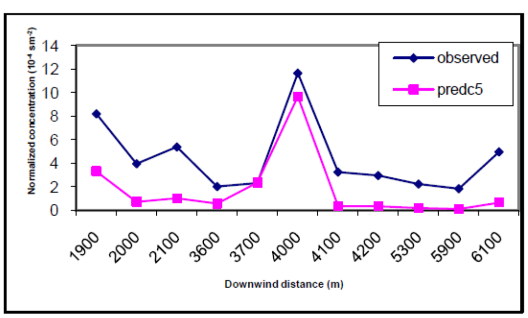


Fig. 1: The observed and predicted concentrations via downwind distance.

Fig. 1 shows the variations of the observed and predicted concentrations (C1-C5) via downwind distance from the source. We conclude that the predictions C1 and C2 are the nearest to the observed concentrations than the other methods.

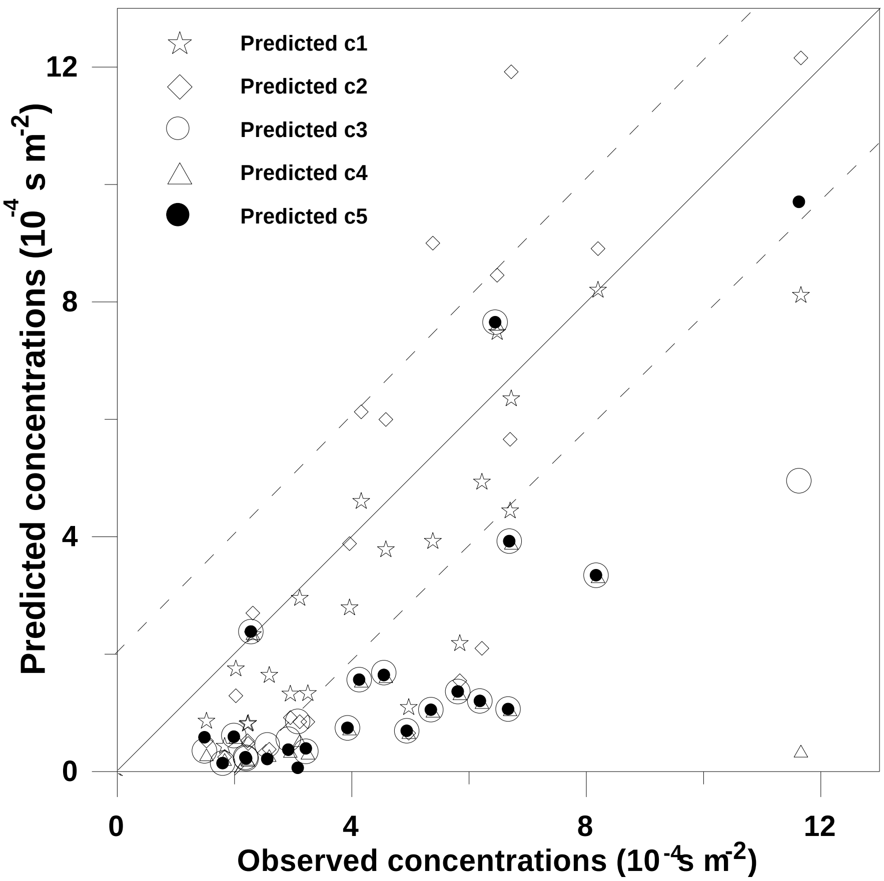


Fig. 2: The relation between the observed and predicted concentrations

Fig. 2 shows that the observed and computed ground-level centerline concentration using intensities parameters α , β , and γ interms of u_* and split sigma theta (σ_θ). We find that the predicted method C1 and C2 lie in factor of two with observed concentration, but the others models (C3, C4 and C5) lie inside factor of four.

The datasets were analyzed subsequently using the following statistical measures (Hanna 1989):

Nmse (normalized mean square error) = $\overline{(C_o - C_p)^2} / C_o C_p$;

Fac2 =fraction of data (%) for $0.5 \le (C_p / C_o) \le 2$;

Cor (Correlation coefficient) = $\overline{(C_o - \overline{C}_o)(C_p - \overline{C}_p)} / \sigma_o \sigma_p$;

Fb (fractional bias) = $\overline{C}_o - \overline{C}_p / 0.5(\overline{C}_o + \overline{C}_p)$;

and **Fs** (fractional standard deviation)= $(\sigma_o - \sigma_p) / 0.5(\sigma_o + \sigma_p)$ where subscripts o and p refer to observed and predicted quantities, respectively, and an over bar indicated an average. These results were compared with those obtained from a Gaussian and non-Gaussian models as shown in Table 4.

Table (5) Statistical indices evaluating the model performance

Model	Nmse	Fac2	Cor	FB	Fs
Predicted C1	0.21	0.68	.87	0.31	0.4
Predicted C2	0.35	0.73	0.8	0.15	0.8
Predicted C3	1.66	0.31	0.68	0.96	0.9
Predicted C4	2.59	0.28	0.38	1.08	1.0
Predicted C5	1.3	0.32	0.78	0.88	1.0

Table 5 shows the statistical approach which indicated that the predicted C1 and C2 methods agreement with the observed data, and the other methods (C3-C5) are far away from the observed data.

Conclusions

The predicted non-Gaussian, Slender and Gaussian models using different shapes of intensity parameters are compared with observed concentrations which are taken from Copenhagen data.
The variations of the observed and predicted concentrations (C1-C5) via downwind distance from the source are studied. We conclude that the predictions C1 and C2 are the nearest to observed data than from the others.
We find that the predicted concentration from non-Gaussian model (C1 method) is inside a factor of two. Also the most predicted concentrations from slender model (C2 method) are inside a factor of two. But the other models (C3 to C5 methods) lie inside a factor of four.

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