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Comparisons between Analytical Solution of the Diffusion Equation, Gaussian Model, Previous Work and Observed Concentrations

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Abstract

This work uses the separation approach to solve the two-dimensional advection-diffusion problem utilizing the wind speed power law and vertical eddy diffusivity. Comparing data on observed Iodine-135 (I^{135}) concentrations with the proposed, Gaussian, prior studies are done. There more agreements are found between the suggested model and the measured I^{135} concentrations than between Gaussian and the earlier research.

Keywords: *Advection-Diffusion; The Separation Approach; Iodine-135; Gaussian and the Earlier Research.*

INTRODUCTION

Different Gaussian and non-Gaussian solutions are included in the atmospheric diffusion equation's analytical solution. Demuth (1978) and Khaled (2014) have derived an analytical solution with a power law of the wind speed and eddy diffusivity under realistic assumptions. In the first part of the 20th century, the majority of the basic theories pertaining to air diffusion were put out Taylor (1921). The combination of advection and diffusion that takes place in the air near the surface of the earth is described mathematically by atmospheric dispersion modeling, which is a term used to characterize pollutant movement in the atmosphere. The advection–diffusion equation that John (2011) studied may be used to characterize the pollutant concentration that is released into the atmosphere. Since Tirabassi et al. (2010) obtained the dispersion from a continuous point source, the advection–diffusion equation has been frequently used in operational atmospheric dispersion models to forecast the mean concentration of pollutants in the planetary boundary layer (PBL). For almost thirty years, researchers Elliot (1961), Malhorta and Cermak (1964), and Marrouf et al. (2013) have recognized that vertical concentration profiles from field and laboratory tests with near-surface point sources releases exhibit non-Gaussian distribution. Essa et al. (2023) compare Gaussian Plume Models with the Analytical Advection-Diffusion Equation under Unstable Conditions. Essa and Hanaa (2023) derive the Gaussian plume model, the Gradient Transport (K) of the advection-diffusion equation, and its applications.

In this study, the concentration is obtained by solving the diffusion equation in two dimensions using variable separation under the fluctuation of wind speed and eddy diffusivity, which in an unstable scenario depend on the vertical height. To determine which model is ideal, statistical analysis is employed.

MATHEMATICAL MODEL

The diffusion equation of pollutants in air can be written in the form by Arya (1995)as follows:

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

Where u is the mean wind directed in the x direction, Ky and Kzare are the crosswind and vertical turbulent eddy diffusivity coefficients of the Planetary Boundary Layer (PBL), and C(x,y.z) is the concentration in the three dimensions x, y, and z directions, respectively. We apply the following boundary conditions to equation (1).

The flux equals zero at the ground surface and the top of PBL as follows:

$$K_z \frac{\partial C}{\partial z} = 0 \qquad at\ z = 0 \qquad (i)$$

$$K_z \frac{\partial C}{\partial z} = 0 \qquad at\ z = h \qquad (ii)$$

The mass continuity is verified as follows:

$$C(0,z) = \frac{Q}{U}\delta(z - h_s) \qquad at\ x = 0 \qquad (iii)$$

Where, δ is the Dirac delta function, h_s is the stack height, h is the PBL height, and Q is the emission rate. After integrating from -∞ to ∞ with regard to y, one obtains:

$$u\frac{\partial}{\partial x}\int_{-\infty}^{\infty} C(x,y,z)dy = K_y \frac{\partial C(x,y,z)}{\partial y}\Big|_{-\infty}^{\infty} + \frac{\partial}{\partial z}\left(K_z \frac{\partial}{\partial z}\right)\int_{-\infty}^{\infty} C(x,y,z)dy \quad (2)$$

Suppose that:

$$\int_{-\infty}^{\infty} C(x,y,z)dy = C_y(x,z) \quad (3)$$

Since $$K_y \frac{\partial C(x,y,z)}{\partial y}\Big|_{-\infty}^{\infty} = 0 \quad (4)$$

By substituting from equations (3) and (4) into equation (2), one can get

$$u\frac{\partial C_y(x,z)}{\partial x} = \frac{\partial}{\partial z}\left(K_z \frac{\partial C_y(x,z)}{\partial z}\right) \quad (5)$$

Remembering that the PBL's height is discredited into N sub-intervals so that, within each interval, u and K_z take on their average values (Tirabassi, et al., 2010). Next, the average values' values are: Equation (5) can only be solved by solving "N" problems of this kind.

$$K_n = \frac{1}{z_{n+1}-z_n}\int_{z_{n+1}}^{z_n} K_Z(z)dz \quad (6)$$

$$u_n = \frac{1}{z_{n+1}-z_n}\int_{z_{n+1}}^{z_n} u(z)dz \quad (7)$$

$$u_n\frac{\partial C_y(x,z)}{\partial x} = K_n\frac{\partial}{\partial z}\left(\frac{\partial C_y(x,z)}{\partial z}\right) \quad (8)$$

$C_y(x, z)$ is called cross-wind integrated concentration of n^{th} sub-interval Tirabassi, et al. (2010). Let the solution of equation (7) using separation variables is in the form.

$$C_y(x,z) = X(x)Z(z)$$

Then equation (8) becomes:

$$uZ(z)\frac{dX(x)}{dx} = K_n\, X(x)\frac{d^2Z(z)}{dz^2} \quad (9)$$

Divided Equation (9) on X(x) Z (z) one gets:

$$\frac{u}{X(x)}\frac{dX(x)}{dx} = \frac{K_n}{Z(z)}\frac{d^2Z(z)}{dz^2} = -\alpha^2 \quad (10)$$

where, α is constant.

The solution of the first term of equation (10) can be written as:

$$\frac{dX(x)}{X} = -\frac{\alpha^2}{u}dx$$

By integration from 0 to x, one gets:

$$Ln\, X = \frac{-a^2}{u}x \quad (11)$$

Then equation (11) becomes:

$$X(x) = e^{-\frac{\alpha^2 x}{u}} \quad (12)$$

The second term of equation (10) can be written as:

$$\frac{d^2Z(z)}{dz^2} + \frac{\alpha^2}{K_n}Z(z) = 0 \quad (13)$$

Then the solution of equation (13) is written in the form:

$$Z(z) = c_1 sin\left(\frac{\alpha}{\sqrt{K_n}}z\right) + c_2 cos\left(\frac{\alpha}{\sqrt{K_n}}z\right) \quad (14)$$

Then the general solution becomes in the form:

$$C_y(x,z) = e^{-\frac{\alpha^2 x}{u}}\left[c_1 sin\left(\frac{\alpha}{\sqrt{K_n}}z\right) + c_2 cos\left(\frac{\alpha}{\sqrt{K_n}}z\right)\right] \quad (15)$$

where c_1 and c_2 are constants. Then applying the first boundary condition (i) one get:

$$e^{-\frac{\alpha^2 x}{u}}\frac{\partial}{\partial z}\left[c_1 sin\left(\frac{\alpha}{\sqrt{K_n}}z\right) + c_2 cos\left(\frac{\alpha}{\sqrt{K_n}}z\right)\right] = 0 \quad at\ z = 0 \quad (16)$$

$$c_1\left(\frac{\alpha}{\sqrt{K_n}}\right)cos\left(\frac{\alpha}{\sqrt{K_n}}z\right) - c_2\left(\frac{\alpha}{\sqrt{K_n}}\right)sin\left(\frac{\alpha}{\sqrt{K_n}}z\right) = 0 \quad at\ z = 0 \quad (17)$$

Substituting by z=0 then one can get:

$$c_1 = 0$$

The general solution can be written as:

$$C_y(x,z) = c_2 e^{-\frac{\alpha^2 x}{u}}cos\left(\frac{\alpha}{\sqrt{K_n}}z\right) \quad (18)$$

Using the boundary condition (ii) one gets:

$$c_2 e^{-\frac{\alpha^2 x}{u}}\frac{\partial}{\partial z}\left(cos\frac{\alpha}{\sqrt{K_n}}z\right) = 0 \quad at\ z = h \quad (19)$$

$$c_2\frac{\alpha}{\sqrt{K_n}}sin\left(\frac{\alpha}{\sqrt{K_n}}z\right) = 0 \quad at\ z = h \quad (20)$$

$$sin\left(\frac{\alpha}{\sqrt{K_n}}h\right) = 0$$

So that $\frac{\alpha h}{\sqrt{K_n}} = n\pi$ (21)

$$\alpha = \frac{n\pi\sqrt{K_n}}{h} \quad (22)$$

Substituting from equation (22) in equation (18) then one gets:

$$C_y(x,z) = c_2 e^{-\frac{n^2\pi^2 k_n x}{h^2}}cos\left(\frac{n\pi}{h}z\right) \quad (23)$$

Using the boundary condition (iii). The equation (23) written as:

$$c_2 cos\left(\frac{n\pi}{h}z\right) = \frac{Q}{u}\delta(z - h_s) \quad atx = 0 \quad (24)$$

Multiplying equation (24) by$cos\left(\frac{n\pi}{h}z\right)$ then one gets:

$$c_2 cos^2\left(\frac{n\pi}{h}z\right) = \frac{Q}{u}\delta(z - h_s)cos\left(\frac{n\pi}{h}z\right) \quad (25)$$

Integrating equation (25) from 0 to h, we have got:

$$\int_0^h c_2\, cos^2\left(\frac{n\pi}{h}z\right) = \int_0^h \frac{Q}{u}\delta(z - h_s)cos\left(\frac{n\pi}{h}z\right) \quad (26)$$

$$\frac{1}{2}c_2\int_0^h\left(1 + cos\left(\frac{2n\pi}{h}z\right)\right)dz = \frac{Q}{u}\delta(z - h_s)cos\left(\frac{n\pi}{h}z\right) \quad (27)$$

$$\frac{1}{2}c_2 h = \frac{Q}{u}cos\left(\frac{n\pi}{h}h_s\right) \quad (28)$$

$$c_2 = \frac{2Q}{uh}cos\left(\frac{n\pi}{h}h_s\right) \quad (29)$$

Substituting by equation (29) in equation (23) one obtains:

$$\frac{C_y(x,z)}{Q} = \frac{2}{uh}cos\left(\frac{n\pi}{h}h_s\right)e^{-\frac{n^2\pi^2 k_n x}{h^2}}cos\left(\frac{n\pi}{h}z\right) \quad (30)$$

Then the concentration at n=0 we have that:

$$C_y(x,z) = \frac{2Q}{uh} \quad (31)$$

At n=1 one can get:

$$C_y(x,z) = \frac{2Q}{uh} cos\left(\frac{\pi}{h}h_s\right) e^{-\frac{\pi^2 k_n x}{h^2}} cos\left(\frac{\pi}{h}z\right) \quad (32)$$

For simplicity the crosswind integrating concentration in the form:

$$\frac{C_y(x,z)}{Q} = \frac{2}{uh}\left[1 + cos\left(\frac{\pi}{h}h_s\right) e^{-\frac{\pi^2 k_n x}{h^2}} cos\left(\frac{\pi}{h}z\right)\right] \quad (33)$$

Then, the concentration in three dimensions is as follows:

$$C(x,y,z) = \frac{1}{\sigma_y\sqrt{2\pi}} e^{-\frac{y^2}{2\sigma_y^2}} C_y(x,z) \quad (34)$$

$$C(x,y,z) = \frac{2Q}{\sigma_y uh\sqrt{2\pi}} e^{-\frac{y^2}{2\sigma_y^2}}\left[1 + cos\left(\frac{\pi}{h}h_s\right) e^{-\frac{\pi^2 k_n x}{h^2}} cos\left(\frac{\pi}{h}z\right)\right] \quad (35)$$

$$C(x,y,z) = \frac{2Q}{\sigma_y uh\sqrt{2\pi}} e^{-\frac{y^2}{2\sigma_y^2}}\left[1 + \sum_1^\infty cos\left(\frac{n\pi}{h}h_s\right) e^{-\frac{n^2\pi^2 k_n x}{h^2}} cos\left(\frac{n\pi}{h}z\right)\right] e^{-\frac{\theta x}{u}} \quad (36)$$

Taking

$$u_n = \beta z^p \quad (37)$$

$$K_n = \gamma z^\epsilon \quad (38)$$

Where, $\beta = 0.16\left(\frac{w_*}{u}\right)^2$ *and* $\gamma = 0.31\left(\frac{w_*}{u}\right)^2$, w_* is the convective vertical velocity and u is the wind speed at 10 m. p *and* $\varepsilon$are the values which depend on the stability conditions.$e^{-\frac{\theta x}{u}}$is the radioactive decay for the specified nuclide, and θ =2.9×10^{-5} is the radioactive decay

Results and Discussion

The observed data of I^{135} isotope concentration was obtained from dispersion as experiments conducted in unstable condition air samples which are taken from IAEA (1980). The observed concentrations data are taken from Essa et al. (2023). The values of Gaussian, previous, previous k-model and proposed concentrations of Iodine-135 (I^{135}) in unstable condition with downwind distance are shown in Table (3) as follows:

Table 1. Power-law exponent 'ϵ' is a function of air stability in urban area.

	A	B	C	D	E	F
ϵ	0.85	0.85	0.80	0.75	0.60	0.40
p	0.15	0.15	0.20	0.25	0.40	0.60

Table 2. Contains the crosswind standard deviation σ_y values through different stabilities.

Stability classes	Values of σ_y
A	$\sigma_y = 0.40x^{0.91}$
B	$\sigma_y = 0.40x^{0.91}$
C	$\sigma_y = 0.36x^{0.86}$
D	$\sigma_y = 0.32x^{0.78}$

Table 3. Gaussian, previous (Essa et al 2023), previous k-model (Essa and Taha 2023) and proposed concentrations for Iodine-135 (I^{135}) in unstable condition with downwind distance.

Test	Downwind distance (m)	Proposed conc. Eqns(36) (Bq/m^3)	Gaussian conc. (Bq/m^3)	previous work conc. (Bq/m^3)	Previous K-model work conc. (Bq/m^3)
1	100	0.0267	0.039975	0.020607	0.027
2	98	0.0345	0.03302	0.044329	0.025
3	136	0.0878	0.082803	0.078956	0.086
4	135	0.2015	0.166257	0.090608	0.182
5	106	0.2737	0.274148	0.331532	0.271
6	186	0.1986	0.107066	0.156713	0.234
7	165	0.4617	0.216606	0.573346	0.367
8	154	0.1246	0.151414	0.125247	0.111
9	106	0.0302	0.044721	0.047909	0.041

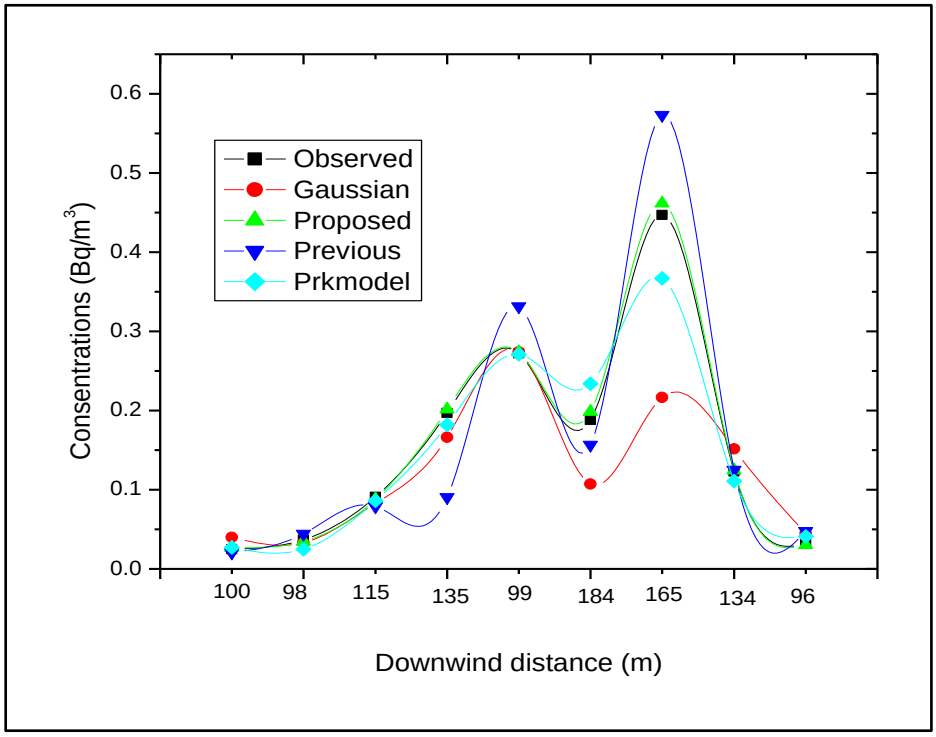


Fig. 1. Relation between Observed, Gaussian, previous, previous k-model and proposed concentrations of (I135) via downwind distance in unstable condition.

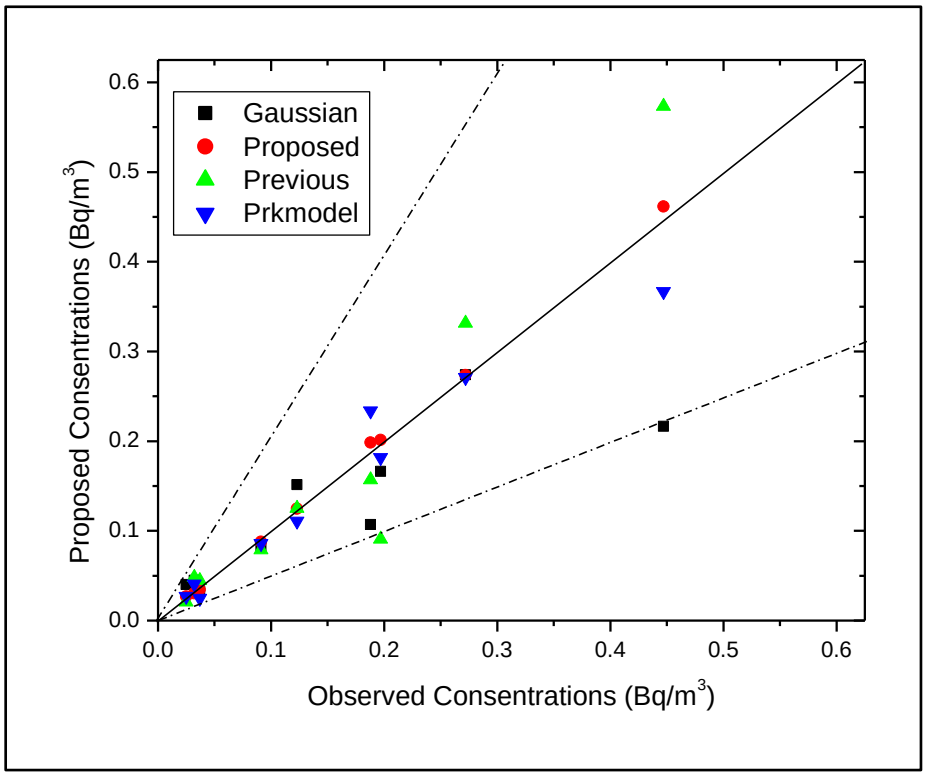


Fig. 2. Relation between Observed, Gaussian, previous, previous k-model and proposed concentrations of (I^{135}) in unstable condition.

Fig. (1) shows that the proposed concentrations is nearer to the observed model than Gaussian , previous and previous k-model. Also, the proposed concentrations are one to one with the observed concentrations model but the Gaussian, previous and the previous k-model.

Statistical Method

Table (4) shows the comparison between Gaussian, predicted and observed concentrations in unstable condition.

Table 4. The comparison between Observed, Gaussian, previous, previous k-model and proposed concentrations in unstable condition

Models	NMSE	FB	COR	FAC2
Proposed. Eq. (36)	0.000686	-0.019	1.00	1.02
Gauss. Eqns.	0.35	0.23	0.84	0.79
previous work	0.14	-0.40	0.95	1.04
Previous K-Model	0.04	0.05	0.98	0.99

Conclusions

The results obtained from the analytical advection diffusion equation are closer to the observed Iodine-135 data under unstable condition than the data obtained with the Gaussian model, previous work and previous k-model. In the Gaussian plume model previous work and previous k- model are located at a factor of two. The correlation factor are near to one for all models. The proposed model and previous k-model are near to zero than Gaussian and previous work.

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