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Theoretical Solution of the Diffusion Equation in Unstable Case

Essa KSM[1]*, Mina AN[2], Hamdy HS[2] and Khalifa AA[2]

[1]*Department of Mathematics and Theoretical Physics, Nuclear Research Centre, Atomic energy Authority, Cairo, Egypt*
[2]*Faculty of science, Beni -Suef University, Egypt*

Abstract

The diffusion equation is solved in two dimensions to obtain the concentration by using separation of variables under the variation of eddy diffusivity which depend on the vertical height in unstable case. Comparing between the predicted and the observed concentrations data of Sulfur hexafluoride (SF6) taken on the Copenhagen in Denmark is done. The statistical method is used to know the best model. One finds that there is agreement between the present, Laplace and separation predicted normalized crosswind integrated concentrations with the observed normalized crosswind integrated concentrations than the predicted Gaussian model.

Keywords: Diffusion equation; Separation of variables; Laplace technique; Gaussian model; Eddy diffusivity

Introduction

The analytical solution of the atmospheric diffusion equation contains different depending on Gaussian and non–Gaussian solutions. An analytical solution with power law of the wind speed and eddy diffusivity with realistic assumption is derived by Demuth [1] and Essa [2]. Most of the fundamental theories of atmospheric diffusion were proposed in the first half of the twentieth century.

The atmospheric dispersion modeling refers to the mathematical description of contaminant transport in the atmosphere is used to describe the combination of diffusion and advection that occurs within the air the earth's surface. The concentration of a contaminant released into the air may therefore be described by the advection – diffusion equation by Stockie JM [3].

The advection – diffusion equation has been widely applied in operational atmospheric dispersion model to predict the mean concentration of contaminants in the planetary boundary layer (PBL) which is obtain the dispersion from a continuous point source by Tiziano T et al. [4].

For nearly thirty years it has been known that vertical concentration profiles from field and laboratory experiments of near-surface point sources releases exhibit non-Gaussian distribution [5-7]. In this work diffusion equation is solved in two diffusivity which depend on the vertical height in unstable case. The statistical technique is used in dimensions to obtain the concentration by using separation of variables under the variation of eddy. The diffusion equation of pollutants in air can be written in the form by Arya [8].

Mathematical Model

$$u\frac{\partial c(x,y,z)}{\partial x}=\frac{\partial}{\partial y}\left(k_y\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial z}\left(k_z\frac{\partial c}{\partial z}\right) \quad (1)$$

where c(x,y.z) is the concentration in the three dimensions x, y and z directions respectively, K_y and K_z are the crosswind and vertical turbulent eddy diffusivity coefficients of the PBL and u is the mean wind oriented in the x direction .

Equation (1) is subjected to the following boundary condition.

$$k_z\frac{\partial c}{\partial z}=0 \text{ at } z=0 \quad (i)$$

$$k_z\frac{\partial c}{\partial z}=0 \text{ at } z=h \quad (ii)$$

$$c(0,z)=\frac{Q}{u}\delta(z-h_s) \text{ at } x=0 \quad (iii)$$

Q is the emission rate, h_s are the stack height, h is the height of PBL and δ is the Dirac delta function.

By integration with respect to y from -∞ to∞, then one gets:

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

Suppose that:

$$\int_{-\infty}^{\infty}c(x,y,z)=c_y(x,z) \quad (3)$$

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:

$$u\frac{\partial c_y(x,y,z)}{\partial x}=\frac{\partial}{\partial z}\left(k_z\frac{\partial c(x,z)}{\partial z}\right) \quad (5)$$

Bearing in mind the dependence of the K_z coefficient, h is the height of PBL is discretized in N sub- intervals in such a manner that inside each interval K_z assume average value. Then the value of the average value is:

$$k_n=\frac{1}{z_{n+1}-z_n}\int_{z_n}^{z_{n+1}}k_z(z)dz$$

***Corresponding author:** Essa KSM, Department of Mathematics and Theoretical Physics, Nuclear Research Centre, Atomic Energy Authority, Cairo, Egypt, Tel: 202-296-4810; E-mail: mohamedksm56@yahoo.com

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The solution of equation (5) is reduced to the solution of "N" problems of the type

$$u\frac{\partial c_y(x,y,z)}{\partial x} = k_n \frac{\partial^2 c_y(x,z)}{\partial z^2} \quad (6)$$

$C_y(x, z)$ is called cross- wind integrated concentration of n^{th} sub-interval.

Let the solution of equation (6) using separation variables is in the form.

c(x,z) =X(x) Z(z)

Then equation (6) becomes:

$$uZ(z)\frac{dX(x)}{x} = k_n X(x)\frac{d^2Z(z)}{dz^2} \quad (7)$$

Divided equation (7) on X(x) Z (z) one gets:

$$\frac{u}{X(x)}\frac{dX(x)}{x} = \frac{k_n}{Z(z)}\frac{d^2Z(z)}{dz^2} = -\alpha^2 \quad (8)$$

Where α is constant. The solution of the first term of equation (8) can be written as:

$$\frac{dX(x)}{x} = -\frac{\alpha^2}{u}x \quad (9)$$

By integration from 0 to x, one gets:

$$\ln X = -\frac{\alpha^2}{u}x \quad (10)$$

Then equation (10) becomes:

$$X(x) = e^{-\alpha^2 x/u} \quad (11)$$

The second term of equation (8) can be written as:

$$\frac{d^2Z(z)}{dz^2} + \frac{\alpha^2}{k_n}Z(z) = 0 \quad (12)$$

Then the solution of equation (12) is written in the form:

$$Z(z) = C_1 \sin\left(\frac{\alpha}{\sqrt{k_n}}z\right) + C_2\cos\left(\frac{\alpha}{\sqrt{k_n}}z\right) \quad (13)$$

Then the general solution becomes in the form:

$$c_y(x,z) = e^{-\frac{\alpha^2}{u}x}\left[C_1 \sin\left(\frac{\alpha}{\sqrt{k_n}}z\right) + C_2\cos\left(\frac{\alpha}{\sqrt{k_n}}z\right)\right] \quad (14)$$

Applying the first boundary condition (i) one gets:

$$e^{-\frac{\alpha^2}{u}}\frac{\partial}{\partial z}\left[C_1 \sin\left(\frac{\alpha}{\sqrt{k_n}}z\right) + C_2\cos\left(\frac{\alpha}{\sqrt{k_n}}z\right)\right] = 0 \text{ at } z = 0 \quad (15)$$

$$C_1\left(\frac{\alpha}{\sqrt{k_N}}\right)\cos\left(\frac{\alpha}{\sqrt{k_n}}z\right) - C_2\left(\frac{\alpha}{\sqrt{k_n}}\right)\sin\left(\frac{\alpha}{\sqrt{k_n}}z\right) = 0 \text{ at } z = 0 \quad (16)$$

Substituting by z = 0 then one can get:

$C_1 = 0$

The general solution can be written as:

$$c_y(x,z) = C_2 e^{-\frac{\alpha^2}{u}x}\cos\left(\frac{\alpha}{\sqrt{k_n}}z\right) \quad (17)$$

Using the boundary condition (ii) one gets:

$$C_2 e^{-\frac{\alpha^2}{u}x}\frac{\partial}{\partial x}\left[\cos\left(\frac{\alpha}{\sqrt{k_z}}z\right)\right] = 0 \text{ at } z = h \quad (18)$$

$$C_2\left(\frac{\alpha}{\sqrt{k_z}}\right)\sin\left(\frac{\alpha}{\sqrt{k_n}}z\right) = 0 \text{ at } z = h \quad (19)$$

$$\sin\left(\frac{\alpha}{\sqrt{k_n}}h\right) = 0 \quad (20)$$

$$\text{So that } \left(\frac{\alpha}{\sqrt{k_n}}h\right) = n\pi \quad (21)$$

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

Substituting from equation (22) in equation (17) then one gets:

$$c_y(x,z) = C_2 e^{-\frac{n^2\pi^2 k_n}{h^2}x}\cos\left(\frac{n\pi}{h}z\right) \quad (23)$$

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

$$C_2\cos\left(\frac{n\pi}{h}z\right) = \frac{Q}{u}\delta(z-h_s) \text{ at } x = 0 \quad (24)$$

Multiplying equation (24) by $\cos(\frac{n\pi}{h}z)$ 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 that:

$$\frac{1}{2}C_2\int_0^h\left(1+\cos\left(\frac{2n\pi}{h}z\right)\right)dz = \frac{Q}{u}\int_0^h \delta(z-h_s)\cos\left(\frac{n\pi}{h}z\right)dz \quad (26)$$

$$\frac{1}{2}C_2 h = \frac{Q}{u}\cos\left(\frac{n\pi}{h}h_s\right) \quad (27)$$

$$C_2 = \frac{2Q}{uh}\cos\left(\frac{n\pi}{h}h_s\right) \quad (28)$$

Substituting by equation (28) in equation (23) one obtains:

$$\frac{c_y(x,z)}{Q} = \frac{2}{uh}\cos\left(\frac{n\pi}{h}h_s\right)\exp\left(-\frac{n^2\pi^2 k_n}{uh^2}x\right)\cos\left(\frac{n\pi}{h}z\right) \quad (29)$$

Then the concentration at n = 0, we have that:

$$c_y(x,z) = \frac{2Q}{uh} \quad (30)$$

At n = 1 one can get:

$$c_y(x,z) = \frac{2Q}{uh}\cos\left(\frac{\pi}{h}h_s\right)\exp\left(\frac{-\pi^2 k_n}{uh^2}x\right)\cos\left(\frac{\pi}{h}z\right) \quad (31)$$

For simplicity the crosswind integrating concentration in the form:

$$\frac{c_y(x,z)}{Q} = \frac{2}{uh}\left[1+\cos\left(\frac{\pi}{h}h_s\right)\exp\left(\frac{-\pi^2 k_n}{uh^2}x\right)\cos\left(\frac{\pi}{h}z\right)\right] \quad (32)$$

Taking $k_n = k_0 w^* z\,(1- z/h_s)$. Where k_0 is the von- Karman constant (k_0~0.4), Z is the vertical height, h_s is the stack height at 115m and w* is the convection velocity scale (Table 1).

Figure 1 shows that the predicted normalized crosswind integrated concentrations values of the present, separation, Laplace and Gaussian predicted models and the observed via downwind distance.

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Run no	Date	PG Stability	K_n	h (m)	W_*	U_{10} (ms^{-1})	Distance (m)	C_y/Q ($10^{-4}\ sm^{-2}$)				
								Observed			Computed	
					w_* (m/s)				Separation	Gaussian	Laplace	Present
1	20-9-78	A	0.14375	1980	1.8	3.34	1900	6.48	7.17	5.16	7,7046931	5.997743
1	20-9-78	A	0.14375	1980	1.8	3.34	3700	2.31	5.13	2.52	3,488227	5.997164
2	26-9-78	C	0.14375	1920	1.8	3.82	2100	5.38	3.7	2.29	4,61996	5.405101
2	26-9-78	C	0.14375	1920	1.8	3.82	4200	2.95	2.18	1.18	2,306918	5.404535
3	19-10-78	B	0.103819	1120	1.3	3.82	1900	8.20	9.8	4.51	8,410968	9.106625
3	19-10-78	B	0.103819	1120	1.3	4.93	3700	6.22	7.53	2.65	3,220596	7.05554
3	19-10-78	B	0.103819	1120	1.3	4.93	5400	4.30	7.44	2.58	1,613861	7.054574
5	9-11-78	C	0.055903	820	0.7	4.93	2100	6.72	9.30	3.63	6,580095	5.738531
5	9-11-78	C	0.055903	820	0.7	6.52	4200	5.84	7.87	2.44	2,044103	7.123884
5	9-11-78	C	0.055903	820	0.7	6.52	6100	4.97	7.86	2.41	1,00388	7.122991
6	30-4-78	C	0.159722	1300	2	6.52	2000	3.96	3.57	1.63	3,751729	7.117371
6	30-4-78	C	0.159722	1300	2	6.68	4200	2.22	2.50	0.82	1,703804	4.517276
6	30-4-78	C	0.159722	1300	2	6.68	5900	1.83	2.20	0.68	1,005404	4.516596
7	27-6-78	B	0.175694	1850	2.2	6.68	2000	6.70	5.27	2.51	5,917179	4.515889
7	27-6-78	B	0.175694	1850	2.2	7.79	4100	3.25	3.52	1.17	2,893086	2.749032
7	27-6-78	B	0.175694	1850	2.2	7.79	5300	2.23	3.06	0.79	2,123662	2.748846
8	6-7-78	D	0.175694	810	2.2	8.11	1900	4.16	8.39	4.20	7,124995	2.640299
8	6-7-78	D	0.175694	810	2.2	8.11	3600	3.02	6.21	2.80	3,123895	5.789855
8	6-7-78	D	0.175694	810	2.2	8.11	5300	1.52	5.89	2.18	1,518876	5.788336
9	19-7-78	C	0.151736	2090	1.9	11.45	2100	4.58	3.43	2.20	4,902058	4.100087
9	19-7-78	C	0.151736	2090	1.9	11.45	4200	3.11	2.77	1.13	2,485021	1.659012
9	19-7-78	C	0.151736	2090	1.9	11.45	6000	2.59	2.49	0.81	1,682239	1.65896

Table 1: Comparison between the predicated and observed crosswind- integrated concentration normalized with the emission source rate at different boundary layer height, downwind distance, wind speed, scaling convection velocity and distance for the different runs.

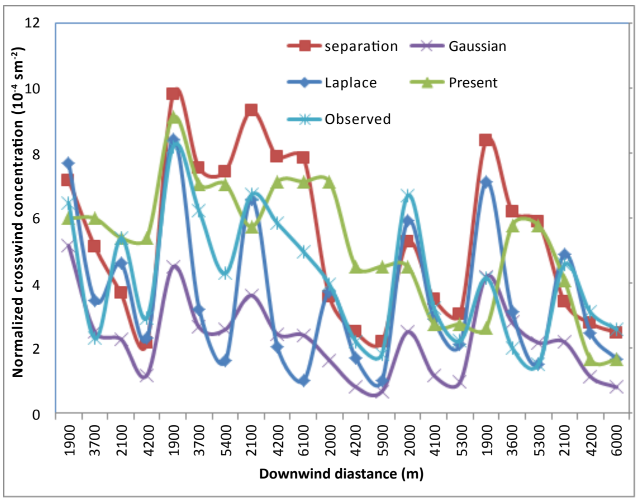

Figure 1: The variation of the three predicted and observed models via down wind distances.

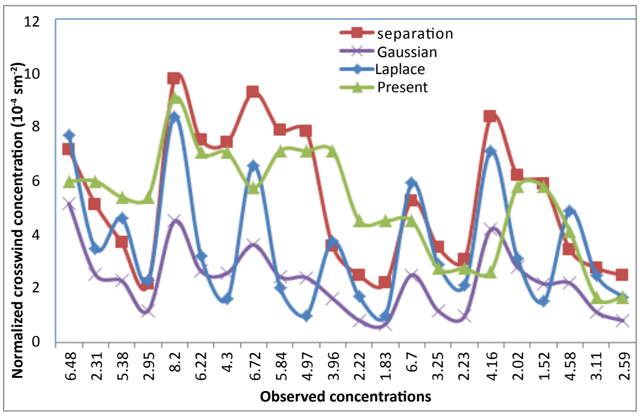

Figure 2: The variation of the three predicted before and present models via observed concentrations.

Figure 2 shows that the predicted normalized crosswind integrated concentrations values of the present, separation, Laplace and Gaussian predicted models via the observed.

From the above two figures, we find that there is agreement between the present, Laplace, Gaussian predicted normalized crosswind integrated concentrations with the observed normalized crosswind integrated concentration than predicted concentration using separation technique.

Model Evaluation Statistics

Now, the statistical method is presented and comparison between predicted and observed results will be offered by Hanna [9]. The following standard statistical performance measures that characterize the agreement between prediction ($C_p = C_{pred}/Q$) and observations ($C_o = C_{obs}/Q$):

$$Fractional\ bias(FB) = \frac{(\bar{C}_o - \bar{C}_p)}{[0.5(\bar{C}_o - \bar{C}_p)]}$$

$$Normalized\ Mean\ Square\ Error\,(\mathrm{NMSE}) = \frac{\overline{(C_p - C_o)^2}}{C_p C_o}$$

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Models	NMSE	FB	COR	FAC2
Present	0.2	-0.21	0.52	1.42
Laplace model	0.18	0.1	0.64	0.95
Separation model	0.22	-0.19	0.6	1.38
Gaussian model	0.58	0.58	0.8	0.59

Table 2: Comparison between Laplace, separation and Gaussian models according to standard statistical performance measure.

$$Correlation\ Coefficient\ (COR) = \frac{1}{N_m}\sum_{i=1}^{N_m}(C_{pi} - \overline{C_p}) \times \frac{(C_{pi} - \overline{C_p})}{(\sigma_p \sigma_o)}$$

$$Factor\ of\ two = 0.5 \le \frac{C_p}{C_o} \le 2.0$$

where σ_p and σ_o are the standard deviations of C_p and C_o respectively. Here the over bars indicate the average over all measurements. A perfect model would have the following idealized performance: NMSE = FB = 0 and COR= FAC2 = 1.0.

Where σ_p and σ_o are the standard deviations of C_p and C_o respectively. Here the over bars indicate the average over all measurements. A perfect model would have the following idealized performance: NMSE = FB = 0 and COR = 1.0 (Table 2).

From the statistical method, we find that the four models are inside a factor of two with observed data. Regarding to NMSE and FB, the present, Laplace and separation predicted models are well with observed data than the Gaussian model. The correlation of present, Laplace and separation predicated model equals (0.52, 0.64 and 0.60 respectively) and Gaussian model equals (0.80).

Conclusion

The crosswind integrated concentration of air pollutants is obtained by using present model by separation technique to solve the diffusion equation in two dimensions. Considering that the eddy diffusivity depends on the vertical distance in unstable case. One finds that there is agreement between the present, Laplace and separation predicted normalized crosswind integrated concentrations with the observed normalized crosswind integrated concentrations than the predicted Gaussian model.

From the statistical method, one finds that the predicted models are inside a factor of two with observed data. Regarding to NMSE and FB, the present, Laplace and separation predicted models are well with observed data than the Gaussian model. The correlation of present, Laplace and separation predicated model equals (0.52, 0.64 and 0.60 respectively) and Gaussian model equals (0.80).

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