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Studying the Effect of the Vertical Eddy Diffusivity on the Solution of the Diffusion Equation

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Abstract: The advection diffusion equation (ADE) is solved in two directions to obtain the crosswind integrated concentration. The solution is solved using Laplace transformation technique and considering the wind speed depends on the vertical height and eddy diffusivity depends on downwind and vertical distances. We compared between the two predicted concentrations and observed concentration data are taken on the Copenhagen in Denmark.

Keywords: Advection Diffusion Equation, Laplace Transform, Predicted Normalized Crosswind Integrated Concentrations.

1.Introduction

The analytical solution of the atmospheric diffusion equation has been containing different shaped depending on Gaussian and non- Gaussian solutions. An analytical solution with power law for the wind speed and eddy diffusivity with the realistic assumption was studied by (Demuth, 1978). The solution has been implemented in the KAPPA-G model (Tirabassi et al., 1986). Lin and (Hildemann, 1997) extended the solution of (Demuth, 1978) under boundary conditions suitable for dry deposition at the ground.The mathematics of atmospheric dispersion modeling is studied by (John, 2011). In the analytical solutions of the diffusion-advection equation, assuming constant along the whole planetary boundary layer (PBL) or following a power law was studied by (Van Ulden, 1978; Pasquill and Smith, 1983; Seinfeld, 1986; Tirabassi et al., 1986; Sharan et al., 1996).

Estimating of crosswind integrated Gaussian and non-Gaussian concentration through different dispersion schemes is studied by (Essa and Fouad, 2011). Analytical solution of diffusion equation in two dimensions using two forms of eddy diffusivities is studied by (Essa and Fouad, 2011).

In this paper the advection diffusion equation (ADE) is solved in two directions to obtain crosswind integrated ground level concentration in unstable conditions. We use Laplace transformation technique and considering the wind speed and eddy diffusivity depends on the vertical height and downwind distance. We compare between observed data from Copenhagen (Denmark) and predicted concentration data using statistical technique.

2. Analytical Method

Time dependent advection – diffusion equation is written as (Arya, 1995).

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

where:

c is the average concentration of air pollution (μg/m^3).

u is the wind speed (m/s).

K_x, k_y and k_z are the eddy diffusivities coefficients along x, y and z axes respectively (m^2/s).

For steady state, taking dc/dt=0 and the diffusion in the x-axis direction is assumed to be zero compared with the advective in the same directions, hence:

$$u\frac{\partial c}{\partial x}=\frac{\partial}{\partial y}\left(k_y\frac{\partial c}{\partial}\right)+\frac{\partial}{\partial z}\left(k_z\frac{\partial c}{\partial}\right) \quad (2)$$

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We must assume that $k_y=k_z=k(x)$. Integrating the equation (2) with respect to y, we obtain the normalized crosswind integrated concentration c_y (x,z) of contaminant at a point (x,z) of the atmospheric advection–diffusion equation is written in the form (Essa et al. 2006) :

$$k\frac{\partial^2 c_{y(x,z)}}{\partial z^2}=u\frac{\partial c_{y(x,z)}}{\partial x} \qquad (3)$$

Equation (3) is subjected to the following boundary condition

1. It is assumed that the pollutants are absorbed at the ground surface

$$k\frac{\partial c_y(x,z)}{\partial z}=-v_g c_y(x,z) \qquad at\ z=0 \qquad (i)$$

where v_g is the deposition velocity (m/s).

2. The flux at the top of the mixing layer can be given by

$$k\frac{\partial c_y(x,z)}{\partial z}=0 \qquad at\ z=h \qquad (ii)$$

3. The mass continuity is written in the form

$$u\, c_y(x,z)=Q\,\delta(z-h) \qquad at\ x=0 \qquad (iii)$$

4. The concentration of the pollutant tends to zero at large distance of the source, i.e.

$$c_y(x,z)=0 \qquad at\ z=\infty \qquad (iv)$$

Applying the Laplace transform on equation (3) to have:

$$\frac{\partial^2\tilde{c}_y(s,z)}{\partial z^2}-\frac{u\,s}{k}\tilde{c}_y(s,z)=-\frac{u}{k}c_y(0,z) \qquad (4)$$

Substituting from equation (iii) in equation (3), we obtain that:

$$\frac{\partial^2\tilde{c}_y(s,z)}{\partial z^2}-\frac{us}{k}\tilde{c}_y(s,z)=-\frac{Q}{k}\delta(z-h) \qquad (5)$$

Where $\tilde{c}_y(s,z)=L_p\{c_y(x,z);\ x\to s\}$, where Lp is the operator of the Laplace transform

$$L\left(\frac{\partial c_y(x,z)}{\partial x}\right)=s\left(\tilde{c}_y(s,z)\right)-c_y(o,z)$$

The nonhomogeneous partial differential equation has a solution in the from:

$$\tilde{c}_y(s,z)=c_1e^{z\sqrt{\frac{su}{k}}}+c_2e^{-z\sqrt{\frac{su}{k}}}+\frac{1}{h\sqrt{suk}}\left(1-e^{-h\sqrt{\frac{su}{k}}}\right) \qquad (6)$$

From the boundary condition (iv), we find $c_1=0$:

$$\tilde{c}_y(s,z)=c_2e^{-z\sqrt{\frac{su}{k}}}+\frac{1}{h\sqrt{suk}}\left(1-e^{-h\sqrt{\frac{su}{k}}}\right) \qquad (7)$$

Using the boundary condition (iii) after taking Laplace transform we get that:

$$\tilde{c}_y(s,z)=\frac{Q}{u\,s}\delta(z-h) \qquad (8)$$

Substituting from equation (8) in equation (7), we get that:

$$c_2=\frac{Q}{u\,s}\delta(z-h) \qquad (9)$$

Substituting from equation (9) in equation (7), we get that:

$$\tilde{c}_y(s,z)=\frac{Q}{us}\delta(z-h)e^{-z\sqrt{\frac{su}{k}}}+\frac{1}{h\sqrt{suk}}\left(1-e^{-h\sqrt{\frac{su}{k}}}\right) \qquad (10)$$

Taking the inverse Laplace transform for the equation (10), we get the normalized crosswind integrated concentration in the form:

$$\frac{c_y(x,z)}{Q}=\frac{h\sqrt{u}}{2\sqrt{\pi k^3x^3}}e^{-\frac{h^2u}{4kx}}+\frac{1}{h\sqrt{\pi x u k}}-\frac{1}{h\sqrt{\pi x u k}}e^{-\frac{h^2u}{4kx}} \qquad (11)$$

In unstable case we take the value of the vertical eddy diffusivity in the form:

$$k(z)=k_v w_* z\ \ (1-z/h) \qquad (12)$$

Substituting from equation (12) in equation (3), we get that:

$$\frac{\partial C_y}{\partial x}=\frac{k_v w_* z\left(1-\frac{z}{h}\right)}{u(z)}\frac{\partial^2 C_y}{\partial^2 z}+\frac{k_v w_*\left(1-\frac{2z}{h}\right)}{u(z)}\left(\frac{\partial C_y}{\partial z}\right) \qquad (13)$$

Applying the Laplace transform on equation (13) respect to x and considering that:

$$\check{c}_y(s,z)=L_p\{c_y(x,z);x\to s\}$$
$$L_p\left(\frac{\partial C}{\partial x}\right)=s\tilde{C}_y(s,z)-C_y(0,z) \qquad (14)$$

Where L_p is the operator of the Laplace transform

Substituting from (14) in equation (13), we obtain that:

$$\frac{\partial^2 \tilde{C}_y(s,z)}{\partial z^2}+\frac{\left(1-\frac{2z}{h}\right)}{\left(z-\frac{z^2}{h}\right)}\frac{\partial \tilde{C}_y(s,z)}{\partial z}-\frac{us}{k_v w_*\left(z-\frac{z^2}{h}\right)}\tilde{C}_y(s,z)=-\frac{u}{k_v w_*\left(z-\frac{z^2}{h}\right)}C_y(0,z) \quad (15)$$

Substituting from (ii) in equation (15) we get:-

$$\frac{\partial^2 \tilde{C}_y(s,z)}{\partial z^2}+\frac{\left(1-\frac{2z}{h}\right)}{\left(z-\frac{z^2}{h}\right)}\frac{\partial \tilde{C}_y(s,z)}{\partial z}-\frac{us}{k_v w_*\left(z-\frac{z^2}{h}\right)}\tilde{C}_y(s,z)=-\frac{Q\delta(z-h_s)}{k_v w_*\left(z-\frac{z^2}{h}\right)} \quad (16)$$

After integrated equation (16) with respect to z, we obtain that:

$$\frac{\partial \tilde{C}_y(s,z)}{\partial z}+\frac{us\ln\left|\frac{z-h}{z}\right|}{k_v w_*}\tilde{C}_y(s,z)=-\frac{Q}{k_v w_* h_s\left(1-\frac{h_s}{h}\right)} \quad (17)$$

Equation (17) is nonhomogeneous differential equation then, above equation has got two solutions, one is homogeneous and other is special solution, in order to solve the homogeneous, we put, $-\frac{Q}{k_v w_* h_s\left(1-\frac{h_s}{h}\right)}=0$ in equation (17), the solution becomes:

$$\frac{\tilde{C}_y(s,z)}{Q}=c_2 e^{-\left(\frac{su\ln\left|\frac{z-h}{z}\right|}{k_v w_*}\right)z} \quad (18)$$

After taking Laplace transform in equation (18) and substitute from (ii), we obtain that:

$$c_2=\frac{1}{us}\delta(z-h_s) \quad (19)$$

Substituting from equation (19) in equation (18) we get that:-

$$\frac{\tilde{C}_y(s,z)}{Q}=\frac{1}{us}e^{-\left(\frac{su\ln\left|\frac{h_s-h}{h_s}\right|}{k_v w_*}\right)z} \quad (20)$$

The special solution of equation (17) becomes:

$$\frac{\tilde{C}_y(s,z)}{Q}=\frac{1}{k_v w_* h_s\left(\frac{h_s}{h}-1\right)}e^{-\left(\frac{su\ln\left|\frac{z-h}{z}\right|}{k_v w_*}\right)z} \quad (21)$$

Then, the general solution of equation (17) is as follows:-

$$\frac{\tilde{C}_y(s,z)}{Q}=\frac{1}{us}e^{-\left(\frac{su\ln\left|\frac{h_s-h}{h_s}\right|}{k_v w_*}\right)z}+\frac{1}{k_v w_* h_s\left(\frac{h_s}{h}-1\right)}e^{-\left(\frac{su\ln\left|\frac{z-h}{z}\right|}{k_v w_*}\right)z} \quad (22)$$

Taking Laplace inverse of equation (22), we get that:-

$$\frac{C_y(x,z)}{Q}=\frac{1}{u\left(x-\frac{u\ln\left|\frac{h_s-h}{h_s}\right|}{k_v w_*}\right)}+\frac{1}{k_v w_* h_s\left(\frac{h_s}{h}-1\right)\left(x+\frac{u\ln\left|\frac{z-h}{z}\right|}{k_v w_*}\right)} \quad (19)$$

Since:

$$L^{-1}(AB)=L^{-1}(A)L^{-1}(B)\ ,\ L^{-1}\left(\frac{1}{s}\right)=1$$

$$,\ L^{-1}(\exp-(as))=\frac{1}{x+a}\ and\ L^{-1}(\exp(as))=\frac{1}{x-a}$$

$L^{-1}$is the operator of the Laplace inverse transform by

(Shamus, 1980).

To get the crosswind integrated ground level concentration, we put z=0 in equation (23), we get that:

$$\frac{C_y(x,0)}{Q} = \frac{1}{u\left(x - \dfrac{u \ln\left|\dfrac{h_s - h}{h_s}\right|}{k_v w_*}\right)} + \frac{1}{k_v w_* h_s\left(\dfrac{h_s}{h} - 1\right)x} \qquad (19)$$

3. Validation

The used data was observed from the atmospheric diffusion experiments conducted at the northern part of Copenhagen, Denmark, under neutral and unstable conditions (Gryning and Lyck, 1984; Gryning et al., 1987). Table (1) shows that the comparison between observed, predicted model 1 and predicted model integrated crosswind ground level concentrations under unstable condition and downwind distance.

Table.1.

Run no.	Stability	Down distance (m)	C_y/Q *10^{-4} (s/m^3)		
			observed	Predicted model 1 $K(x) = 0.16 (\sigma_w^2/u)\, x$.	Predicted model 2 $K(z)= k_v w_* z\ (1-z/h)$
1	**Very unstable (A)**	**1900**	6.48	**8.95**	5.01
1	**Very unstable (A)**	**3700**	2.31	**4.64**	2.62
2	**Slightly unstable (C)**	**2100**	5.38	**6.28**	4.36
2	**Slightly unstable (C)**	**4200**	2.95	**3.14**	2.26
3	**Moderately unstable (B)**	**1900**	8.2	**10.92**	5.01
3	**Moderately unstable (B)**	**3700**	6.22	**6.30**	2.61
3	**Moderately unstable (B)**	**5400**	4.3	**8.30**	1.80
5	**Slightly unstable (C)**	**2100**	6.72	**9.47**	4.50
5	**Slightly unstable (C)**	**4200**	5.84	**9.01**	2.27
5	**Slightly unstable (C)**	**6100**	4.97	**12.19**	1.57
6	**Slightly unstable (C)**	**2000**	3.96	**5.30**	4.35
6	**Slightly unstable (C)**	**4200**	2.22	**2.53**	2.21
6	**Slightly unstable (C)**	**5900**	1.83	**1.98**	1.60
7	**Moderately unstable (B)**	**2000**	6.7	**8.11**	4.57
7	**Moderately unstable (B)**	**4100**	3.25	**3.96**	2.32
7	**Moderately unstable (B)**	**5300**	2.23	**3.06**	1.81
8	**Neutral (D)**	**1900**	4.16	**10.31**	4.89
8	**Neutral (D)**	**3600**	2.02	**5.45**	2.68
8	**Neutral (D)**	**5300**	1.52	**4.37**	1.85
9	**Slightly unstable (C)**	**2100**	4.58	**6.86**	4.34
9	**Slightly unstable (C)**	**4200**	3.11	**3.43**	2.26
9	**Slightly unstable (C)**	**6000**	2.59	**2.40**	1.60

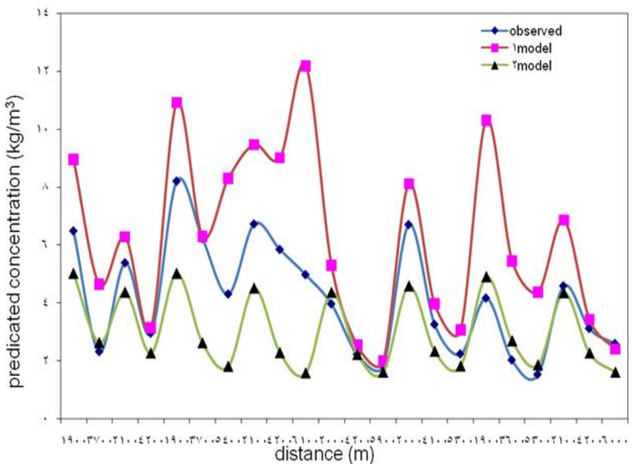

Fig. 1. The variation of the two predicted and observed models via downwind distances.

Fig. (1) Shows that the predicted normalized crosswind integrated concentrations values of the model 2are good to the observed data than the predicted of model 1.

Fig. (2) Shows that the predicted data of model 2 is nearer to the observed concentrations data than the predicted data of model 1.

From the above figures, we find that there are agreement between the predicted normalized crosswind integrated concentrations of model 2 depends on the vertical height with the observed normalized crosswind integrated concentrations than the predicted model 1 which depends on the downwind distance.

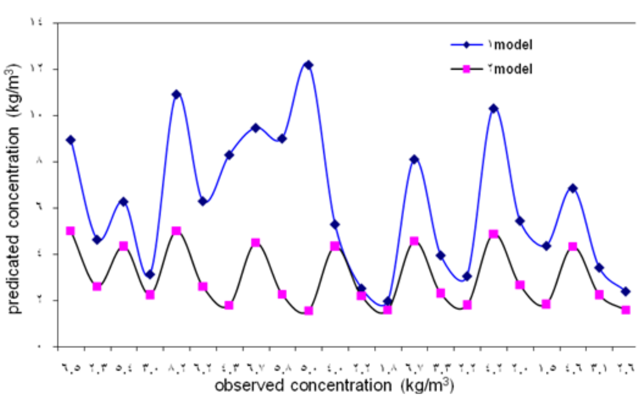

Fig. 2. The variation between the predicted models and observed concentrations data.

4. Statistical method

Now, the statistical method is presented and comparison between predicted and observed results will be offered by (Hanna, 1989).The following standard statistical performance measures that characterize the agreement between prediction ($C_p=C_{pred}/Q$) and observations ($C_o=C_{obs}/Q$):

$$Fractional\ Bias\ (FB) = \frac{(\overline{C_o}-\overline{C_p})}{[0.5(\overline{C_o}+\overline{C_p})]}\ \text{Normalized Mean Square Error (NMSE)} = \frac{\overline{(C_p-C_o)^2}}{\overline{(C_pC_o)}}\ Correlation\ Coefficient\ (COR) = \frac{1}{N_m}\sum_{i=1}^{N_m}(C_{pi}-\overline{C_p}) \times \frac{(C_{oi}-\overline{C_o})}{(\sigma_p\sigma_o}\ Factor\ of\ Two\ (FAC2) = 0.5 \le \frac{C_p}{C_o} \le 2.0$$

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 = 1.0.

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

$$Fractional\ Bias\ (FB) = \frac{(\overline{C_o}-\overline{C_p})}{[0.5(\overline{C_o}+\overline{C_p})]}$$

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

$$Factor\ of\ Two\ (FAC2) = 0.5 \le \frac{C_p}{C_o} \le 2.0$$

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 = 1.0.

Table. 2. Comparison between our two models according to standard statistical Performance measure

Models	**NMSE**	**FB**	**COR**	**FAC2**
Predicated model 1	**0.30**	**-0.40**	**0.78**	**1.56**
Predicated model 2	**0.26**	**0.32**	**0.67**	**0.80**

From the statistical method, we find that the two models are inside a factor of two with observed data. Regarding to NMSE and FB, the predicted two models are good with observed data the correlation of predicated model 1 equals (0.78) and model 2 equals (0.67).

4. Conclusion
5.

We find that the predicted crosswind integrated concentrations of the two models are inside a factor of two with observed concentration data. One finds that there is agreement between the predicted normalized crosswind integrated concentrations of model 2 depends on the vertical height with the observed normalized crosswind integrated concentrations than the predicted model 1 which depends on the downwind distance.

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