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

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Author's contribution

This whole work was carried out by the author KSME.

Original Research Article

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ABSTRACT

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

Keywords: Advection diffusion equation; laplace transform; predicted normalized crosswind integrated concentrations.

1. INTRODUCTION

The analytical solution of the atmospheric diffusion equation contains different shapes depending on Gaussian and non- Gaussian solutions. An analytical solution with power law of the wind speed and eddy diffusivity with the realistic assumption was studied by Demuth [1]. The solution implemented in the KAPPA-G model by Tirabassi [2] and Lin and Hildemann [3] extended the solution of Demuth [1] under boundary conditions suitable for dry deposition at the ground. The mathematics of atmospheric dispersion modeling was studied by John [4]. In the analytical solutions of the diffusion-advection equation, assuming constant wind speed along the whole planetary boundary layer (PBL) or following a power

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law was studied by Van Ulden [5]; Pasquill and Smith [6]; Seinfeld [7]; Tirabassi [2] and Sharan [8].

Estimating of crosswind integrated Gaussian and non-Gaussian concentration through different dispersion schemes is studied by Essa [9]. Analytical solution of diffusion equation in two dimensions using two forms of eddy diffusivities is studied by Essa [10].

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. Comparison between observed data from Copenhagen (Denmark) and predicted concentration data using statistical technique was presented.

2. ANALYTICAL METHOD

Time dependent advection – diffusion equation is written by Arya [11] as:

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

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 diffusivity 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 advection in the same directions, hence:

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

Let us assume that $k_y = k_z = k(x)$
Integrating equation (2) with respect to y by Essa [12]:

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

Equation (3) is subjected to the following boundary conditions as:

1-The pollutants are absorbed at the ground surface i.e.

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

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

2-There is no flux at the top of the mixing layer, i.e.

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

3-The mass continuity is written in the form:

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

Where δ is the Dirac delta function, Q is the source strength and "h" is mixing height.
4-The concentration of the pollutant tends to zero at large distance of the source, i.e.

$$c_y(x,z) = 0 \qquad \text{at } z=\infty \tag{iv}$$

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

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

where $\tilde{c}_y(s,z)=L_p\{c_y(x,z)$; x→s}, where L_p is the operator of the Laplace transform
Substituting from equation (iii) in equation (4), to get:

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

$$L\left[\frac{\partial c_y(x,z)}{\partial x}\right]=s\{\tilde{c}_y(s,z)\}-c_y(0,z)$$

The nonhomogeneous partial differential equation (5) has a solution in the form:

$$\tilde{c}_y(s,z)=c_1 e^{z\sqrt{\frac{su}{k}}}+c_2 e^{-z\sqrt{\frac{su}{k}}}+\frac{1}{h\sqrt{suk}}\left(1-e^{-h\sqrt{\frac{su}{k}}}\right) \tag{6}$$

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

$$\tilde{c}_y(s,z)=c_2 e^{-z\sqrt{\frac{su}{k}}}+\frac{1}{h\sqrt{suk}}\left(1-e^{-h\sqrt{\frac{su}{k}}}\right) \tag{7}$$

Using the boundary condition (iii) after taking Laplace transform,

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

$$L\left[\frac{\partial c_y(x,z)}{\partial x}\right]=s\{\tilde{c}_y(s,z)\}-c_y(0,z) \tag{8}$$

Substituting from equation (8) in equation (7),

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

Substituting from equation (9) in equation (7),

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

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

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

<u>In unstable case</u>: Taking the value of the vertical eddy diffusivity in the form:

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

Substituting from equation (12) into equation (3),

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

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

To have:

$$L_p\left(\frac{\partial C}{\partial x}\right) = s\tilde{C}_y(s,z) - C_y(0,z) \quad (14)$$

Substituting from (14) in equation (13),

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

Substituting from (ii) in equation (15),

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

Integrating equation (16) with respect to z, to have:

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

Equation (17) is nonhomogeneous differential equation. The homogeneous solution of (17) is given by:

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

After taking Laplace transform for equation (18) and substituting from (ii),

$$c_2=\frac{1}{u\,s}\delta(z-h_s) \tag{19}$$

Substituting from equation (19) in equation (18),

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

The special solution of equation (17) becomes:

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

Then, the general solution of equation (17) is a combination between the two solutions (20) and (21) as:

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

Taking Laplace inverse transform of equation (22) using Shamus [13].

$$\frac{C_y(x,z)}{Q}=\frac{1}{u\left(x-\frac{u\,\ln\left|\frac{h_s-h}{h_s}\right|}{k_v w_*}\right)}+\frac{1}{k_v w_* h_s\left(\frac{h_s}{h}-1\right)\left(x+\frac{u\,\ln\left|\frac{z-h}{z}\right|}{k_v w_*}\right)} \tag{23}$$

This is the concentration of pollutant at any point (x,z)

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

$$\frac{C_y(x,0)}{Q} = \frac{1}{u\left(x - \frac{u \ln\left|\frac{h_s - h}{h_s}\right|}{k_v w_*}\right)} + \frac{1}{k_v w_* h_s \left(\frac{h_s}{h} - 1\right) x} \tag{24}$$

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 by Gryning and Lyck [14]; Gryning [15]. Table (1) shows that the comparison between observed, predicted model "1" and predicted model "2" integrated crosswind ground level concentrations under unstable condition and downwind distance.

Table 1. The comparison between observed, predicted model "1" and predicted model "2" integrated crosswind ground level concentrations under unstable condition and downwind distance

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

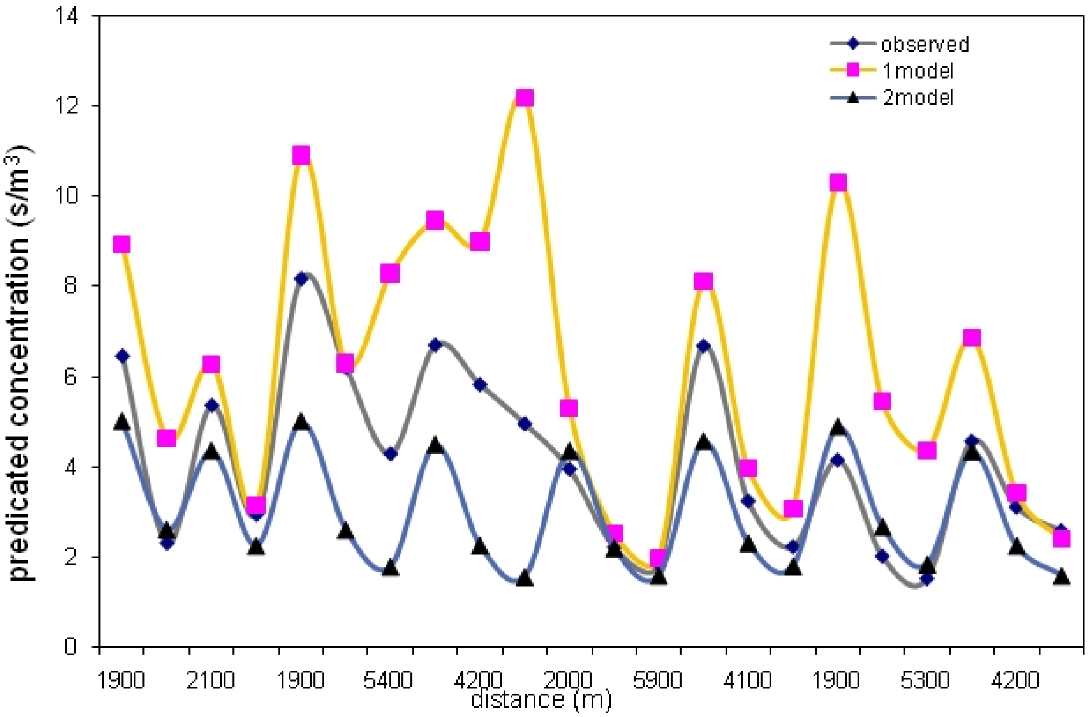

Fig. 1. The variation of the two predicted and observed models via downwind distances.

Fig. (1) Shows 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 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" that depends on the downwind distance.

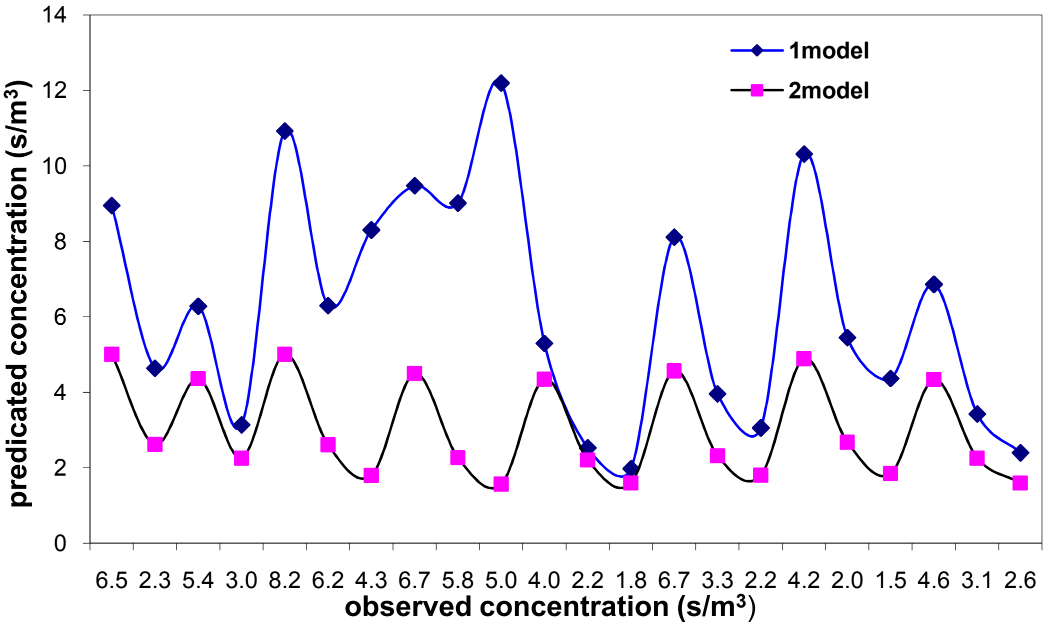

Fig. 2.The variation between the predicted models and observed concentrations data.

4. STATISTICAL METHOD

Now, the statistical method is presented and comparison between predicted and observed results was offered by Hanna [16].The following standard statistical performance measures that characterize the agreement between prediction (Cp =Cpred/Q) and observations (Co=Cobs/Q):

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

Where σ_p and $\sigma_o$are the standard deviations of C_p and C_o respectively. Here the over bars indicate the average over all measurements. A perfect model has the following idealized performance: NMSE = FB = 0 and COR = 1.0.

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

$$FractionalBias\ (FB) = \frac{(\overline{C_o} - \overline{C_p})}{\left[0.5(\overline{C_o} + \overline{C_p})\right]}$$

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

$$FactorofTwo(FAC2) = 0.5 \leq \frac{C_p}{C_o} \leq 2.0$$

Where σ_p and σ_o are the standard deviations of C_p and C_o respectively. 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, it is evident 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).

5. CONCLUSIONS

The predicted crosswind integrated concentrations of the two models are inside a factor of two with observed concentration data. 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. This means that the vertical eddy diffusivity depends on the vertical height "z" than downwind distance "x". Also in the further work we will take the eddy diffusivity depends on the vertical height and downwind distance.

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COMPETING INTERESTS

Author has declared that no competing interests exist.

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