

## **Studying the effect of vertical eddy diffusivity on the solution of diffusion equation**

### **Abstract**

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

*Key Words: Advection Diffusion Equation, Laplace Transform, Predicted Normalized Crosswind Integrated Concentrations.*

### **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, 1978). The solution implemented in the KAPPA-G model (Tirabassi et al., 1986) and (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 was studied by (John, 2011). In the analytical solutions of the diffusion-advection equation, assuming constant wind speed 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 and Sharan et al., 1996).

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

In this paper the advection diffusion equation (ADE) is solved in two dimensions to obtain crosswind integrated ground level concentration in unstable conditions. We

use Laplace transformation technique and considering the wind speed and eddy diffusivity depend on the vertical height and downwind distance. Comparison between observed data from Copenhagen (Denmark) and predicted concentration data using statistical technique was presented.

### 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 ( $\mu\text{g}/\text{m}^3$ ).

$u$  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 ( $\text{m}^2/\text{s}$ ).

End in the  $x$ -axis direction is assumed to be zero and in the  $y$ -axis direction is assumed to be zero. The direction, hence:

$$K_x \frac{\partial^2 c}{\partial x^2} = 0 \quad \text{and} \quad K_y \frac{\partial^2 c}{\partial y^2} = 0 \quad (2)$$

that, assume  $K_z = K(x)$  with respect to  $y$ , (Essa et al. 2006) :

$$u \frac{\partial c}{\partial x} = \frac{\partial}{\partial z} \left( K \frac{\partial c}{\partial z} \right) + \frac{\partial^2 c}{\partial x^2} \quad (3)$$

Equation (3) is subjected to the following boundary condition

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

$$K \frac{\partial c_y(x, z)}{\partial z} = -v_g c_y(x, z) \quad \text{at } z = 0 \quad (i)$$

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

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

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

3-The mass continuity is written in the form:-

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

Where  $\delta$  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.

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

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

$$\frac{\partial^2 \phi_y(s,z)}{\partial z^2} - \frac{us}{k} \phi_y(s,z) = -\frac{u}{k} c_y(0,z) \quad (4)$$

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

Substituting from equation (iii) in equation (4), to get:

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

$$L\left(\frac{\partial c_y(x,z)}{\partial x}\right) = s(\phi_y(s,z)) - c_y(0,z)$$

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

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

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

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

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

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

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

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

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

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

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

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

**In unstable case:** 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),

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

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

$$\tilde{c}_y(s, z) = L_p\{c_y(x, z); x \rightarrow s\}$$

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),

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

Substituting from (ii) in equation (15),

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

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

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

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

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

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

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

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

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

The special solution of equation (17) becomes:

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

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

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

Taking Laplace inverse transform of equation (22) using Shamus (1980),

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

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):

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

### **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 "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)	$C_y/Q \cdot 10^{-4} \text{ (s/m}^3\text{)}$		
			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 vb	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

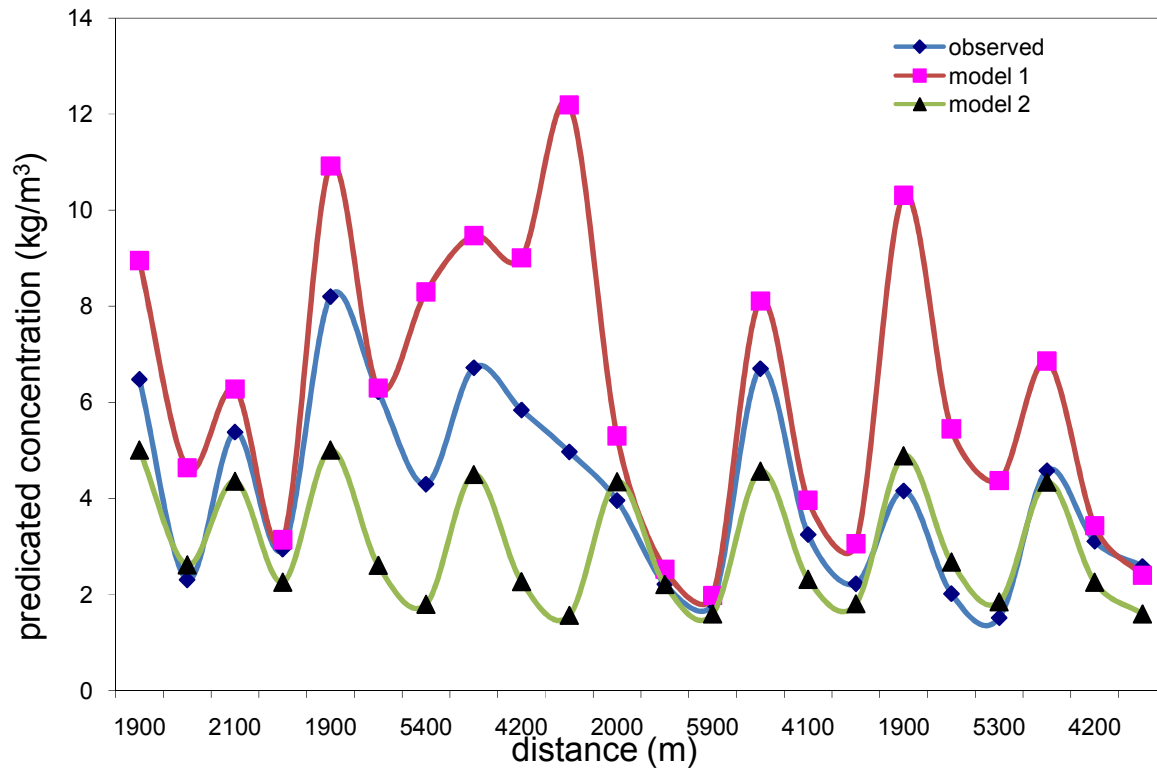


Fig. 1 The variation of the two predicted and observed models via downwind distances

Fig. (1) Shows the predicted normalized crosswind integrated concentrations values of the model 2 are 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.

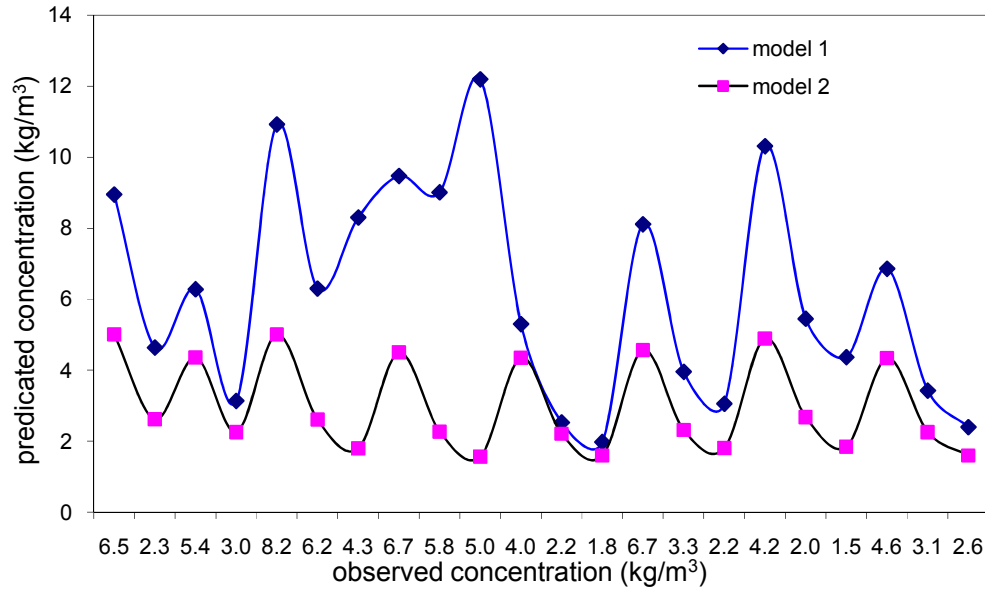


Fig. 2 The variation between the predicted models and observed concentrations data.

### Statistical method

Now, the statistical method is presented and comparison between predicted and observed results was 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)

$$= \frac{(\overline{C_o} - \overline{C_p})}{0.5(\overline{C_o} + \overline{C_p})} \text{ Normalized Mean Square Error (NMSE)}$$

$$= \frac{(\overline{C_p - C_o})^2}{(\overline{C_p C_o})} \text{ Correlation Coefficient (COR)}$$

$$= \frac{1}{N_m} \sum_{i=1}^{N_m} (C_{pi} - \overline{C_p}) \times \frac{(C_{oi} - \overline{C_o})}{(\sigma_p \sigma_o)} \text{ Factor of Two (FAC2)}$$

$$= 0.5 \leq \frac{C_p}{C_o} \leq 2.0$$

Where  $\sigma_p$  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.

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

<b>Models</b>	<b>NMSE</b>	<b>FB</b>	<b>COR</b>	<b>FAC2</b>
<b>Predicated model 1</b>	<b>0.30</b>	<b>- 0.40</b>	<b>0.78</b>	<b>1.56</b>
<b>Predicated model 2</b>	<b>0.26</b>	<b>0.32</b>	<b>0.67</b>	<b>0.80</b>

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).

## **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.

## References

- Arya, S. P. (1995) "Modeling and parameterization of near – source diffusion in weak wind" J. Appl. Met. 34, 1112-1122.
- Demuth, C. (1978) "A contribution to the analytical steady solution of the diffusion equation" Atmos. Environ., 12, 1255.
- Gryning S. E., and Lyck E., (1984), "Atmospheric dispersion from elevated sources in an urban area: Comparison between tracer experiments and model calculations", J. Climate Appl. Meteor., 23, pp. 651-660.
- Gryning S.E., Holtslag, A.A.M., Irwin, J.S., Sivertsen, B., (1987), "Applied dispersion modeling based on meteorological scaling parameters", Atmos. Environ. 21 (1), 79-89.
- Hanna S. R., 1989, "confidence limit for air quality models as estimated by bootstrap and Jackknife resembling methods", Atmos. Environ. 23, 1385-1395.
- John M. Stockie, (2011), The Mathematics of atmospheric dispersion modeling. Society for Industrial and Applied Mathematics. Vol. 53. No.2 pp. 349-372.
- Essa K. S. M., Maha S. EL-Qtaify, (2006) "Diffusion from a point source in an urban Atmosphere" Meteorol. Atmos. Phys., 92, 95-101.
- Essa K. S. M., and E. A. Found , (2011), "Estimated of crosswind integrated Gaussian and Non-Gaussian concentration by using different dispersion schemes". Australian Journal of Basic and Applied Sciences, 5(11): 1580-1587.
- Essa K. S. M., A. N. Mina and Mamdouh Higazy, (2011), Analytical Solution of diffusion equation in two dimensions using two forms of eddy diffusivities, Rom. Journal. Phys., VI.56, Nos.9-10, P. 1228-1240, Bucharest.
- Lin, J.S. and Hildemann L.M. (1997), "A generalized mathematical scheme to analytically solve the atmospheric

diffusion equation with dry deposition, Atmos. Environ". 31, 59-

- Pasquill, F., Smith, F.B., (1983) "Atmospheric Diffusion 3<sup>rd</sup> edition". Wiley, New York, USA
- Seinfeld, J.H., (1986), Atmospheric Chemistry and physics of Air Pollution. Wiley, New York.
- Shamus (1980) "Theories and examples in Mathematics for Engineering and Scientific".
- Sharan, M., Singh, M.P., Yadav, A.K. (1996), " Mathematical model for atmospheric dispersion in low winds with eddy diffusivities as linear functions of downwind distance". Atmospheric Environment 30, 1137-1145.
- Tirabassi, T., Tagliazucca, M., Zannetti, P., KAPPAG, (1986) "A non-Gaussian plume dispersion model". JAPCA 36, 592-596.
- Van Ulden A.P., Hotslag, A. A. M., (1978), "Estimation of atmospheric boundary layer parameters for diffusion applications". Journal of Climate and Applied Meteorology 24, 1196- 1207.
- Zannetti, P., KAPPAG, (1986) "A non-Gaussian plume dispersion model". JAPCA 36, 592-596.