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TIME DEPENDENT ADVECTION DIFFUSION EQUATION IN TWO DIMENSIONS

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ABSTRACT

In this work, the advection diffusion equation is solved in two dimensional space (x, z) which depends on time using Laplace transform technique to evaluate crosswind integrated of pollutant concentration per emission rate. Two schemes of the eddy diffusivities to get two models (1&2) were applied to evaluate crosswind integrated concentration per emission rate according to boundary layer parameterization. Terabassi et al model was taken as a reference model. Comparison between these two models, reference model and observed data were carried out. The observed Copenhagen data set is composed of SF_6 tracer due to dispersion experiments carried out in Northern Copenhagen, 20 minutes averaged measured concentrations were used.One finds all models were inside a factor of two. Model 2 and reference model were better when compared with the observed data than model 1 with respect to NMSE. The two models are better with respect to FB than reference model. All models were good with respect to the correlation coefficient except model 1.Finally, we can conclude that predicted (C_p) crosswind-integrated concentration normalized with the emission source rate for all models were inside a factor of two with observed data (C_o). Crosswind- integrated concentration normalized with the emission source rate for all models were good when compared with observed data via downwind distances.

Keywords: Laplace transform technique, Crosswind concentration, Advection equation, Downwind distance, Analytical solution, Eddy diffusivities.

Contribution/ Originality

This study contributes in the existing literature with solving the advection diffusion equation in two dimensional spaces (x, z) which depends on time using Laplace transform technique to evaluate crosswind integrated of pollutant concentration per emission rate. Two schemes of the eddy diffusivities to get two models (1&2) were applied to evaluate crosswind integrated concentration per emission rate according to boundary layer parameterization. Terabassi et al model was taken as a reference model. Comparison between these two models, reference model

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and observed data were carried out. This study uses new modeling proposal for estimation of crosswind-integrated concentration normalized with the emission source rate.

1. INTRODUCTION

Atmospheric dispersion modeling refers to the mathematical description of contaminant transport in the atmosphere. The term dispersion in this context was used to describe the combination of diffusion (due to turbulent eddy motion) and advection (due to wind) that occurs within the earth's surface air. The concentration of a contaminant released into the air may therefore be described by the advection – diffusion equation, which is a second –order partial differential equation (PDE) of parabolic type. Analytical and approximate solutions for the atmospheric dispersion problem have been derived under wide range of simplifying assumptions, as well as various boundary conditions and parameter dependencies. These analytical solutions are especially useful to engineers and environmental scientists who study pollutant transport, since they allow parameter sensitivity and source estimation studies to be performed [1].

Both our scientific understanding and technical developments have been greatly increased by the use of empirical, analytical and numerical models to predict air pollution concentration in the atmosphere. For this purpose, the advection – diffusion equation has been largely applied in operational atmospheric dispersion models. In principal, from this equation it is possible to predict mean concentrations of contaminants in the planetary boundary layer due to a continuous point source by given appropriate boundary and initial conditions plus knowledge of the mean wind velocity and concentration turbulent fluxes [2].

Many turbulent dispersion studies are related to the specification of these turbulent fluxes to allow the solution of the averaged advection –diffusion equation.

The main objective of this work is to derive the advection diffusion equation in two dimensional spaces (x, z) which depends on time using Laplace transform technique to evaluate crosswind integrated of pollutant concentration per emission rate. Boundary parameterizations were applied in two models of the eddy diffusivity coefficient. Comparison between these two models, reference model [3] and observed data were carried out. The observed Copenhagen data set is composed of SF_6 tracer from dispersion experiments carried out in northern Copenhagen, 20 minutes averaged measured concentrations were used.

1.1. Analytical Solution

A typical problem in air pollution is to seek the solution for the cross-wind (y direction) integrated of pollutant concentration for a continuous source of pollution in the from Tiziano, et al. [3]:-

$$\frac{\partial \bar{C}(x,z,t)}{\partial t} + u\frac{\partial \bar{C}(x,z,t)}{\partial x} = \frac{\partial}{\partial z}\left(K\frac{\partial \bar{C}(x,z,t)}{\partial z}\right) \tag{1}$$

where $\bar{C}$ denotes the crosswind integrated of pollutant concentration, Kis the vertical turbulent eddy diffusivity coefficient of the PBL into N sub- intervals [3] and u is the mean wind oriented in the x direction.

Equation (1) is subjected to the following boundary condition

u C(x, z, t) =Q δ (z-h_s) at x=0 (i)

C(x, z, t) = 0 at t = 0 (ii)

C(x, z, t) = 0 at z → ∞ (iii)

K ∂ C(x, z, t)/ ∂ z = 0 at z=0,h (iv)

Q is the emission rate, h_s is the stack height, h is the height of PBL and δ is the Dirac Delta function. 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 [3]:-

$$K_n = \frac{1}{z_{n+1} - z_n} \int_{z_n}^{z_{n+1}} K_z(z) dz \quad (2)$$

Therefore the solution (1) is reduced to the solution of N problems of the type:

$$\frac{\partial \bar{C}(x,z,t)}{\partial t} + u \frac{\partial \bar{C}(x,z,t)}{\partial x} = K_n \frac{\partial^2 \bar{C}_n(x,z,t)}{\partial z^2} \quad (3)$$

For n=1,2,3 .., N-1, where $\bar{C} = \bar{C}_n$ denotes the concentration at the n^{th} sub-interval [3].

Applying the Laplace transform on equation (3) to x, t, we get that:-

$$\frac{\partial^2 \tilde{\tilde{C}}_n(s,z,p)}{\partial z^2} - \left(\frac{p+us}{K_n}\right) \tilde{\tilde{C}}_n(s,z,p) = -\frac{Q}{K_n} \delta(z - h_s) \quad (4)$$

where $\tilde{\tilde{C}}(s,z,p)$ = $L_p\{\bar{C}$ (x, z, t); x→s, t→p}, and Lp is the operator of the Laplace transform.

The Equation (4) nonhomogeneous partial differential equation, the general solution of this equation consists of two solutions, the first solution is homogeneous equation and the second is special solution, to solve the homogeneous solution from equation (4), Let:

- (Q / k) δ (z- h_s) has a solution in the from Spiegel [4]:

$$\tilde{\tilde{C}}(s,z,p) = c_1 e^{z\sqrt{\frac{p+us}{K}}} + c_2 e^{-z\sqrt{\frac{p+us}{K}}} \quad (5)$$

Substituting from (iii) on equation (3), we get that:-

c_1=0

$$\tilde{\tilde{C}}(s,z,p) = c_2 e^{-z\sqrt{\frac{p+us}{K}}} \quad (6)$$

Applying the Laplace transform on equation (i) to x, t, we get that:-

$$\frac{\tilde{\tilde{C}}(s,z,p)}{Q}=\frac{1}{u\,s\,p}\delta(z-h_s) \tag{7}$$

Compared between (6) and (7), we get:-

$$c_2=\frac{Q}{u\,s\,p}e^{z\sqrt{\frac{p}{K}}}\delta(z-h_s) \tag{8}$$

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

$$\begin{aligned}\tilde{\tilde{C}}(s,z,p)&=\frac{Q}{u\,s\,p}\delta(z-h_s)\,e^{+z\sqrt{\frac{p}{K}}}e^{-z\sqrt{\frac{p+us}{K}}}\Rightarrow\\ \tilde{\tilde{C}}(s,z,p)&=\frac{Q}{u\,s\,p}\exp\left(-h_s\sqrt{\frac{p+us}{K}}+h_s\sqrt{\frac{p}{K}}\right)\end{aligned} \tag{9}$$

Where, $e^x=1+x+\frac{x^2}{2!}+\cdots\cdots,\cdots\cdots$

$$(a+x)^n=a^n+\binom{n}{1}a^{n-1}x+\binom{n}{2}a^{n-2}x^2+\cdots\, and$$

$$\binom{n}{k}=\frac{n!}{k!(n-k)!}$$

$$\frac{\tilde{\tilde{C}}_n(s,z,p)}{Q}=\frac{1}{u\,s\,p}\left(1+h_s\left(\sqrt{\frac{p}{K_n}}-\sqrt{\frac{p+us}{K_n}}\right)\right)= \tag{10}$$

$$\frac{1}{u\,s\,p}-\frac{1}{2}\frac{h_s}{p^{\frac{3}{2}}\sqrt{K}}$$

Applying the Laplace inverse transform on equation (10), we get that:-

$$\frac{\bar{C}_n(x,z,t)}{Q}=\frac{1}{u\,\pi^2 x\,t}-\frac{h_s\sqrt{t}}{\sqrt{K_n\pi}} \tag{11}$$

where $L^{-1}\left(\frac{1}{s^n}\right)=\frac{t^{n-1}}{\Gamma(n)},L^{-1}\left(s^n\right)=0\,and\;L^{-1}\left(\frac{1}{s}\right)=1$

To solve the second special solution from equation (4) have that:-

$$\frac{\tilde{\tilde{C}}_n(s,z,p)}{Q}=\frac{-\delta(z-h_s)}{K_n\left(D^2-\left(\frac{p+u\,s}{K_n}\right)\right)} \tag{12}$$

Then, the general solution to this form is given by:

$$e^{mz}\left(\int e^{-mz}R(z)dz\right)$$

Where: $D=\frac{\partial}{\partial z}\because y(z)=\frac{R(z)}{D-m}$

Then, the general solution to this form is given by:

The solution to equation (12) is given by:

$$\frac{\tilde{\tilde{C}}_n(s,z,p)}{Q}=\frac{1}{2\sqrt{K_n(p+us)}}\left(\exp\left(\frac{(z-2h+h_s)}{(z+h_s)}\right)\right) \quad (13)$$

Substituting from equation (8) on equation (12) and applying the Laplace inverse transform on equation (13), we get that

$$\frac{\bar{C}_n(x,z,t)}{Q}\frac{1}{2\sqrt{K_n\pi t}}\left(\exp\left(\frac{(z-2h+h_s)}{(z+h_s)}\right)\right) \quad (14)$$

Summation the equations (14) and (11) we have the general solution of equation (2) on the form:

$$\frac{\bar{C}_n(x,z,t)}{Q}=\frac{1}{u\pi^2xt}-\frac{h_s\sqrt{t}}{\sqrt{K_n\pi}}+\frac{1}{2\sqrt{K_n\pi t}}\left(\exp\left(\frac{(z-2h+h_s)}{(z+h_s)}\right)\right) \quad (15)$$

1.2. Boundary Layer Parameterization

We applied a parameterization proposed by Troen and Marth [5] as presented in Pleim and Chang [6].

The vertical eddy diffusivity (in model 1) [7] in near and stable conditions ($\frac{Z_i}{L}\geq 10$), in the form:

$$K_z=\frac{ku_*z\left(1-z/z_i\right)^2}{\theta_h\left(z/L\right)}$$

$$where\ \theta_h=\left(1-16z/L\right)^{-1/2}$$

Where k is the Von Karman constant (k~0.4), Zi is the boundary layer height, z is the height at 115 m and w* is the convective velocity scale. The vertical eddy diffusivity (in model 2) during convective ($\frac{z_i}{L}\geq 10$) the frication velocity (u_*) as scaling velocity in the form:

$$K_z=kw_*z\left(1-z/z_i\right)$$

1.3. Validation and Experimental Data

A preliminary evaluation of the performances of the two models (with the boundary layer parameterization proposed), using the Copenhagen data set were applied [7, 8]. The Copenhagen data set is composed of tracer SF_6 data from dispersion experiments carried out in northern Copenhagen. .In practical, we used 20 minutes averaged measured concentration. In Table (1) Comparison between the predicted and observed crosswind- integrated concentration normalized with the emission source rate at different boundary layer height, distance, wind speed and scaling convection velocity for the different runs.

In figure (1) scatter plot of observed (C_o) versus predicted (C_p) crosswind- integrated concentration normalized with the emission source rate. Points between dashed lines are in a factor of two. Figure (2), shows comparison between distance and crosswind- integrated concentration normalized with the emission source rate, we find most points inside factor of two.

In Table (2) Comparison between three models according to standard statistical performance were applied.

Table-1. Comparison between predicted 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 different runs.

Run no.	Z_i(m)	U (m/s)	X(m)	w_* (m/s)	C/Q(10^{-4}s/m^2)			
					observed	Model 1	Model 2	Ref. model [3]:
1	1980	3.34	1900	1.8	6.48	5.8	5.4	5.50
1	1980	3.34	3700	1.8	2.31	1.3	2.0	3.10
2	1920	3.82	2100	1.8	5.38	5.7	6.2	3.60
2	1920	3.82	4200	1.8	2.95	3.2	3.4	1.20
3	1120	3.82	1900	1.3	8.2	1.3	6.2	6.20
3	1120	4.93	3700	1.3	6.22	4.4	4.1	5.40
3	1120	4.93	5400	1.3	4..3	6.3	2.2	3.30
5	820	4.93	2100	0.7	6.72	6.7	7.7	5.80
5	820	6.52	4200	0.7	5.84	4.1	5.5	3.60
5	820	6.52	6100	0.7	4.97	3.2	3.2	2.30
6	1300	6.52	2000	2	3.96	3.1	4.2	2.80
6	1300	6.68	4200	2	2.22	2.1	3.6	1.20
6	1300	6.68	5900	2	1.83	2.5	2.3	1.40
7	1850	6.68	2000	2.2	6.7	5.1	5.7	6.40
7	1850	7.79	4100	2.2	3.25	2.8	4.0	5.20
7	1850	7.79	5300	2.2	2.23	3.5	3.1	2.10
8	810	8.11	1900	2.2	4.16	4.4	5.4	3.20
8	810	8.11	3600	2.2	2.02	1.2	1.1	2.01
8	810	8.11	5300	2.2	1.52	1.3	2.7	1.40
9	2090	11.45	2100	1.9	4.58	2.8	6.1	2.20
9	2090	11.45	4200	1.9	3.11	2.8	4.3	3.00
9	2090	11.45	6000	1.9	2.59	3.5	3.7	1.62

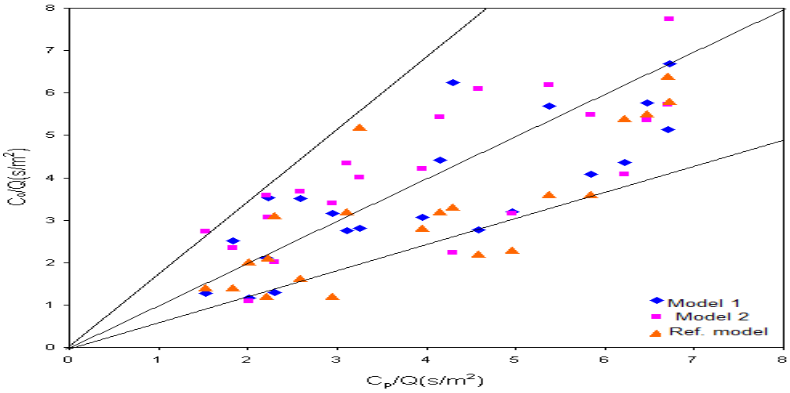

Fig-1. Scatter plot of observed (C_o) and predicted (C_p) crosswind – integrated concentration normalized with the emission source rate

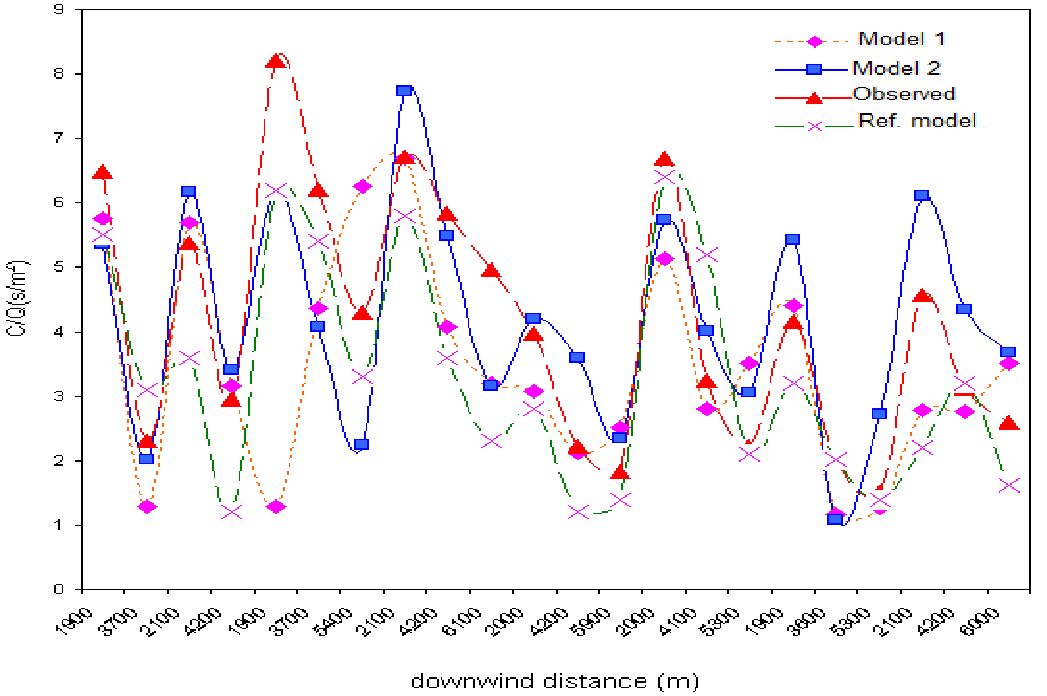

Fig-2. Comparison between downwind distance and concentration crosswind - integrated concentration normalized with the emission source rate

1.4. Statistical Method

Now, the statistical method is presented and comparison among analytical, statically and observed results will be applied [9]. The following standard statistical performance measures characterizes the agreement between models predictions (Cp=Cpred/Q) and observations (Co=Cobs/Q):

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

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

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

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

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 (Nm). A perfect model would have the following idealized performance:

NMSE = FB = 0 and COR = FAC2 = 1.0

Table-2. Comparison between different models according to standard statistical performance measure

Models	NMSE	FB	COR	FAC2
Model 1	0.23	0.17	0.54	0.91
Model 2	0.08	-0.01	0.77	1.08
Ref. model	0.13	0.23	0.83	0.81

From the statistical, we find that all models are within a factor of two. Model (2) and Ref. model were better when compared with observed data than model (1) with respect to NMSE. The two models are better with respect to FB than Ref. model. All models were good with respect to the correlation coefficient except model1.

2. CONCLUSION

We solve the advection diffusion equation in two dimensional spaces (x, z) depending on time. Using Laplace transform technique to find crosswind integrated of pollutant concentration per emission rate, we applied two schemes of the eddy diffusivities to get two models. Terabassi et al model was taken as a reference model. Comparison between these two models, reference model and observed data were carried out. The observed Copenhagen data set is composed of SF_6 tracer due to dispersion experiments carried out in Northern Copenhagen, 20 minutes averaged measured concentrations were used.

One finds all models were inside a factor of two. Model 2 and reference model were better when compared with the observed data than model 1 with respect to NMSE. The two models are better with respect to FB than reference model. All models were good with respect to the correlation coefficient except model 1.

Finally, we can conclude that predicted (C_p) crosswind-integrated concentration normalized with the emission source rate for all models were inside a factor of two when compared with observed data (C_o). Crosswind- integrated concentration normalized with the emission source rate were good for all models when compared with observed data via downwind distances.

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