

The Concentration of Pollutants in Two Dimensional with Constant and Variable Vertical Eddy Diffusivity

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Abstract— Fourier and Hankel transformations are used to solve the advection-diffusion equation in two-dimensional to get normalized cross-wind integrated concentration of pollutants at the surface of the earth with constant and variable eddy diffusivity respectively. The pollutants are assumed to be totally reflected on the ground. The results of predicted model were compared with measuring observed data from Copenhagen, Denmark in unstable condition and the Research Reactor at Enshas, Egypt in neutral condition.

Keywords— Fourier and Hankel transformations; advection-diffusion equation; Eddy diffusivity.

I. INTRODUCTION

Air pollutants are transported, dispersed or deposited by meteorological and topographical conditions. The atmospheric advection-diffusion equation had long been used to describe the transport of pollutant in a turbulent atmosphere was studied by [1]. An analytical solution was fundamental importance which was described with physical phenomena was studied by [2]. References [3-5], used analytical solution to examine the accuracy and performance of the numerical solutions. Reference [6], studied the performance of a unified formal analytical solution for the simulation of atmospheric diffusion problems under stable conditions.

Reference [7], studied simple fractional differential equation models for the steady state spatial distribution of concentration of a non-reactive pollutant in Planetary Boundary Layer (PBL). They found that fractional derivatives models perform better than the traditional Gaussian model.

Reference [8], investigated mathematical model for dispersion of air pollutants in moderated winds taking the diffusion in vertical height direction and advection along the mean wind considering the eddy diffusivity and wind speed was assumed constant. Reference [9], studied the Influence of Eddy Diffusivity Variation on the Atmospheric Diffusion Equation.

Reference [10], investigated an analytical dispersion Model for sources in the atmospheric surface layer with dry deposition to the ground Surface. Also studying the variation of eddy diffusivity

on the behavior of advection-diffusion equation was studied by [11].

Fourier and Hankel transformations are used to solve the advection-diffusion equation in two-dimensional to get normalized cross-wind integrated concentration of pollutants at the surface of the earth with constant and variable Eddy diffusivity respectively. The pollutants are assumed to be totally reflected on the ground. The results of predicted model were compared with measuring observed data of Sulfur Hexa-fluoride SF₆ from Copenhagen, Denmark in unstable conditions and the Research Reactor at Enshas, Egypt in neutral conditions.

II. MATHEMATICAL TREATMENTS

The advection diffusion equation can be written as follows:

$$u \frac{\partial C_y(x, z)}{\partial x} = \frac{\partial}{\partial z} \left(k_z \frac{\partial C_y(x, z)}{\partial z} \right) \quad (1)$$

where $C_y(x, z)$ is the crosswind integrated concentration of pollutants, u is the downwind velocity in m/s and k_z is vertical eddy diffusivity that is taken as a function in downwind distance " x ".

Equation (1) is solved under the boundary conditions as follows:

The null flux condition of contaminants on the ground surface and the top at the vertical height are used:

$$\frac{\partial C_y}{\partial z} = 0 \text{ at } z = 0, h \quad (2a)$$

where " h " is the height of the planetary boundary layer (PBL). In addition, the mass continuity of the source with emission rate " Q " at the height of the source " h_s ".

$$uC_y(0, z) = Q\delta(z - h_s) \quad (2b)$$

A. Constant Eddy Diffusivity

By using Fourier transform, one can find that

$$\widehat{C}_y(x, \xi) = \int_{-\infty}^{\infty} e^{-iz\xi} C_y(x, z) dz \quad (3)$$

and

$$\frac{\partial \widehat{C}_y}{\partial x} = \int_{-\infty}^{\infty} e^{-iz\xi} \frac{\partial C_y}{\partial x} dz \quad (4)$$

From (1) one can get,

$$\frac{\partial \widehat{C}_y}{\partial x} = \frac{k_z}{u} \int_{-\infty}^{\infty} e^{-iz\xi} \frac{\partial^2 C_y}{\partial z^2} dz \quad (5)$$

Using integration by parts twice and the boundary conditions one find

$$\frac{\partial \widehat{C}_y}{\partial x} = -\frac{k_z}{u} \xi^2 \widehat{C}_y(x, \xi) \quad (6)$$

The solution of (6) is easy to get

$$\widehat{C}_y(x, \xi) = A e^{-\frac{\xi^2}{u} \int_0^x k_z dx} \quad (7)$$

using the boundary condition (2b) then

$$A = \frac{Q}{u} e^{-ih_s \xi} \quad (8)$$

Substituting from (8) into (7) we get

$$\widehat{C}_y(x, \xi) = \frac{Q}{u} \exp \left[-ih_s \xi - \frac{\xi^2}{u} \int_0^x k_z dx \right] \quad (9)$$

Assuming the vertical eddy diffusivity as follows [8]:

$$k_z = \frac{0.16 \sigma_w^2}{u} x \quad (10)$$

Then, we can rewrite (8) in the form:

$$\widehat{C}_y(x, \xi) = \frac{Q}{u} \exp \left[-ih_s \xi - \frac{0.08 \sigma_w^2 \xi^2}{u^2} x^2 \right] \quad (11)$$

Consider the inverse Fourier transformation as follows:

$$C_y(x, z) = \int_{-\infty}^{\infty} e^{iz\xi} \widehat{C}_y(x, \xi) d\xi \quad (12)$$

Then, (11) will be

$$C_y(x, z) = \frac{Q \sqrt{\pi}}{\sqrt{0.08 \sigma_w x}} \exp \left[-\frac{u^2 (h_s - z)^2}{0.32 \sigma_w^2 x^2} \right] \quad (13)$$

B. Variable Eddy Diffusivity

Assuming the vertical eddy diffusivity as follows:

$$k_z = \alpha z \quad (14)$$

Then (1) can be written as

$$z \frac{\partial^2 C_y}{\partial z^2} + \frac{\partial C_y}{\partial z} - \frac{u}{\alpha} \frac{\partial C_y}{\partial x} = 0 \quad (15)$$

Changing the independent variable z to ξ by the substitution $\xi = z^{\frac{1}{2}}$ then, (15) will be

$$\xi^2 \frac{\partial^2 C_y}{\partial \xi^2} + \xi \frac{\partial C_y}{\partial \xi} - \frac{4u}{\alpha} \xi^2 \frac{\partial C_y}{\partial x} = 0 \quad (16)$$

Equation (16) can be further simplified to:

$$\frac{\partial^2 C_y}{\partial \xi^2} + \frac{1}{\xi} \frac{\partial C_y}{\partial \xi} - \frac{4u}{\alpha} \frac{\partial C_y}{\partial x} = 0 \quad (17)$$

Equation (17) can be solved for $C(x, \xi)$ by using Hankel transform which is defined as

$$\mathcal{H}_m \{f(z)\} = \tilde{f}(s) \equiv \int_0^{\infty} f(z) J_m(sz) z dz$$

where the Bessel differential operator is defined as

$$\Delta_m f(z) \equiv \frac{d^2 f(z)}{dz^2} + \frac{1}{z} \frac{df(z)}{dz} - \left(\frac{m}{z}\right)^2 f(z)$$

which has the Hankel transform given by

$$\mathcal{H}_m \{\Delta_m f(z)\} \equiv -s^2 \tilde{f}(s)$$

Applying the Hankel transform to (17)

$$\mathcal{H}_0 \left\{ \Delta_0 C_y = \frac{4u}{\alpha} \frac{\partial C_y}{\partial x} \right\} \quad (18)$$

we get

$$-s^2 \tilde{C}_y = \frac{4u}{\alpha} \frac{\partial \tilde{C}_y}{\partial x} \quad (19)$$

Equation (19) has the solution,

$$\tilde{C}_y(x, s) = A \exp \left[-\frac{\alpha}{4u} x s^2 \right] \quad (20)$$

using the boundary condition (2b) then

$$\tilde{C}_y(x, s) = \frac{Q}{2u} J_0 \left(s h_s^{\frac{1}{2}} \right) \exp \left[-\frac{\alpha}{4u} x s^2 \right] \quad (21)$$

Now assuming the inverse Hankel Transformation

$$\begin{aligned} \mathcal{H}_0^{-1} \{ \tilde{C}_y(x, s) \} &= C_y(x, \xi) \\ &\equiv \int_0^{\infty} \tilde{C}_y(x, s) J_0(s\xi) s ds \quad (22) \end{aligned}$$

Then we will have

$$C_y(x, \xi) = \frac{Q}{\alpha x} \exp \left(-\frac{u(h_s + \xi^2)}{\alpha x} \right) I_0 \left(\frac{2u\xi h_s^{\frac{1}{2}}}{\alpha x} \right) \quad (23)$$

By using the substitution $\xi = z^{\frac{1}{2}}$

$$C_y(x, z) = \frac{Q}{\alpha x} \exp \left(-\frac{u(h_s + z)}{\alpha x} \right) I_0 \left(\frac{2u\sqrt{h_s z}}{\alpha x} \right) \quad (24)$$

And finally the concentration can be written as

$$C(x, y, z) = \frac{Q}{\sqrt{2\pi\sigma_y \alpha x}} \exp \left(-\frac{u(h_s + z)}{\alpha x} \right) I_0 \left(\frac{2u\sqrt{h_s z}}{\alpha x} \right) e^{-\frac{y^2}{2\sigma_y^2}} \quad (25)$$

III. RESULTS AND DISCUSSION

The used data was obtained from experiments carried out under unstable condition at the Northern part of Copenhagen, Denmark [12-13]. Table I shows that the meteorology, predicated and observed crosswind-integrated normalized concentration at different downwind distances. Also we used data from Research Reactor at Enshas, Egypt in neutral condition where assume ($\sigma_y = 0.32x^{0.78}$) of standard

deviation in crosswind are taken from [14]. The Comparison between the predicted and observed concentration at different downwind distance, wind speed in neutral condition in Table II.

TABLE I. COMPARISON BETWEEN THE PREDICATED AND OBSERVED CROSSWIND- INTEGRATED NORMALIZED CONCENTRATION AT DIFFERENT DOWNWIND DISTANCE, WIND SPEED, MIXING HEIGHT AND CONVECTIVE VERTICAL VELOCITY FOR THE DIFFERENT RUNS.

Run No.	Date	PG Stability	h (m)	w_* (ms^{-1})	U_{10} (ms^{-1})	Distance (m)	$C_y/Q(10^{-4} \text{ sm}^{-2})$	
							Observed	Predicted Constant k_z
1	20-9-78	A	1980	0.83	2.1	1900	6.48	6.28
1	20-9-78	A	1980	0.83	2.1	3700	2.31	3.24
2	26-9-78	C	1920	1.07	4.9	2100	5.38	4.39
2	26-9-78	C	1920	1.07	4.9	4200	2.95	2.21
3	19-10-78	B	1120	0.68	2.4	1900	8.20	7.62
3	19-10-78	B	1120	0.68	2.4	3700	6.22	3.95
3	19-10-78	B	1120	0.68	2.4	5400	4.30	2.71
5	9-11-78	C	820	0.71	3.1	2100	6.72	6.59
5	9-11-78	C	820	0.71	3.1	4200	5.84	3.33
5	9-11-78	C	820	0.71	3.1	6100	4.97	2.30
6	30-4-78	C	1300	1.33	7.2	2000	3.96	3.71
6	30-4-78	C	1300	1.33	7.2	4200	2.22	1.78
6	30-4-78	C	1300	1.33	7.2	5900	1.83	1.27
7	27-6-78	B	1850	0.87	4.1	2000	6.70	5.66
7	27-6-78	B	1850	0.87	4.1	4100	3.25	2.79
7	27-6-78	B	1850	0.87	4.1	5300	2.23	2.16
8	6-7-78	D	810	0.72	4.2	1900	4.16	7.10
8	6-7-78	D	810	0.72	4.2	3600	2.02	3.82
8	6-7-78	D	810	0.72	4.2	5300	1.52	2.61
9	19-7-78	C	2090	0.98	5.1	2100	4.58	4.78
9	19-7-78	C	2090	0.98	5.1	4200	3.11	2.42
9	19-7-78	C	2090	0.98	5.1	6000	2.59	1.69

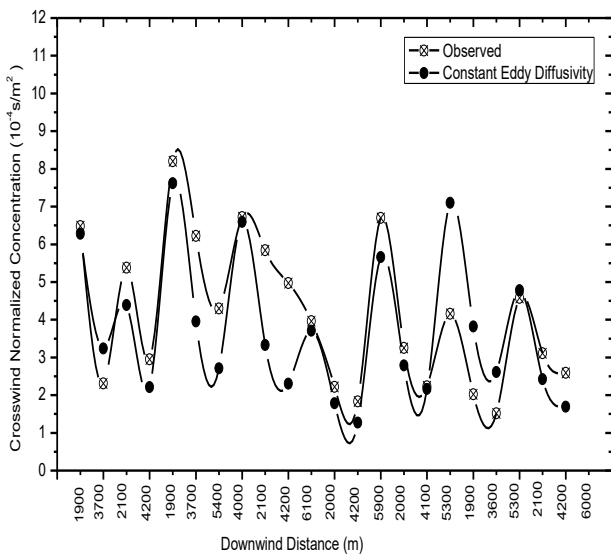


Fig. 1. Observed and proposed crosswind integrated concentration (10^{-4} m/s^2) with constant k_z vs downwind distance (m)

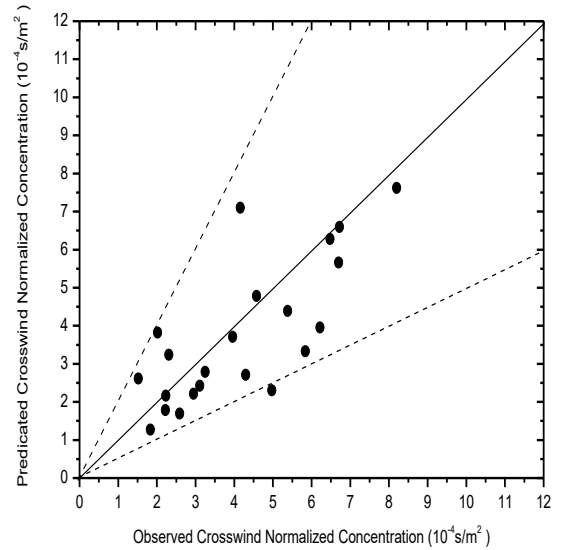


Fig. 2. Proposed concentration with constant k_z vs observed concentration

TABLE II. SHOWS THE COMPARISON BETWEEN THE PREDICATED AND OBSERVED CONCENTRATION AT DIFFERENT DOWNWIND DISTANCE IN NEUTRAL CONDITION.

Run	Distance (m)	Observed C (Bq/m3)	Predicted C(constant k_z) (Bq/m3)	Predicted C(variable k_z) (Bq/m3)
1	100	4.1	2.95	3.69
2	110	3.8	2.85	3.62
3	120	3.8	2.74	3.52
4	130	3.7	2.62	3.39
5	140	3.4	2.50	3.25
6	150	3.2	2.39	3.10
7	160	3.1	2.28	2.96
8	170	3.0	2.18	2.81
9	180	2.9	2.09	2.68
10	190	2.7	2.00	2.55
11	200	2.4	1.92	2.42
12	300	1.4	1.34	1.50
13	400	0.5	1.02	1.01

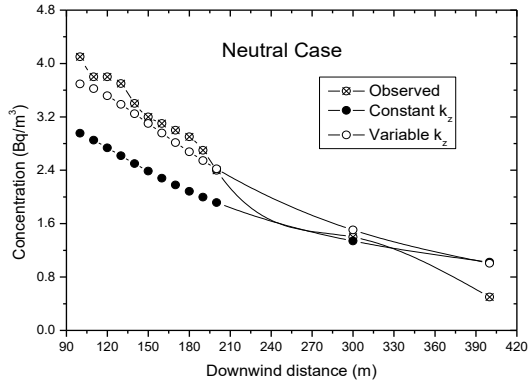


Fig. 3. Observed and proposed concentration at constant and variable k_z in neutral condition via downwind distance (m)

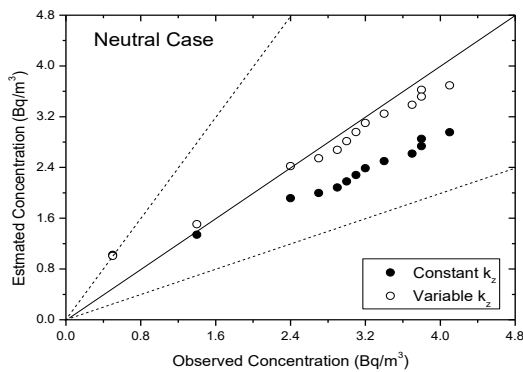


Fig. 4. Observed and proposed concentration at constant and variable k_z downwind distance (m)

From the two figures we can see that most of the predicted data are one to one with the observed concentrations.

IV. MODEL EVALUATION STATISTICS RESULTS

To evaluate the model accuracy we used the following statistical technique that characterizes the agreement between the predicted and observed concentrations. These measures are discussed by [14] defined as:

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

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

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

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

where σ_p and σ_o are the standard deviations of predicted ($C_p=C_{pred}/Q$) and observed ($C_o=C_{obs}/Q$) concentration respectively. The over-bar indicates the average value. The perfect model must have the following performances: NMSE = FB = 0 and COR=FAC2 = 1.0.

TABLE III. SHOWS STATISTICAL EVALUATION OF THE PRESENT MODELS

Model	NMSE	FB	COR	FAC2
Model with constant k_z (Copenhagen)	0.12	-0.11	0.76	1.11
Model with constant k_z (Enshas)	0.11	0.27	0.99	0.76
Model with variable k_z (Enshas)	0.01	0.04	1.00	0.96

V. CONCLUSION

We used Fourier and Hankel transformations are used to solve the advection-diffusion equation in two-dimensional to get normalized cross-wind integrated concentration of pollutants at the surface of the earth with constant and variable Eddy diffusivity respectively. The pollutants are assumed to be totally reflected on the ground. The results of predicted model were compared with measuring observed data from Copenhagen, Denmark unstable condition and the Research Reactor at Enshas, Egypt in neutral condition.

One finds that the present predicted model using Fourier method with constant vertical eddy diffusivity has good agreement with observed data on Research Reactor at Enshas and Copenhagen in Denmark. Also, the present predicted model with variable vertical eddy diffusivity has good agreement with observed data than another predicted with constant vertical eddy diffusivity on Copenhagen.

From the statistical analysis, one finds that the analytical model is within factor of 2 (FAC2) with the observed data. The NMSR and FB are near to zero with Variable k_z in Enshas Than Constant k_z in Copenhagen and Enshas. Also, the COR and FAC2 are near to one.

REFERENCES

The template will number citations consecutively within brackets [1]. The sentence punctuation follows the bracket [2]. Refer simply to the reference number, as in [3]—do not use “Ref. [3]” or “reference [3]” except at the beginning of a sentence: “Reference [3] was the first .”

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