

The Influence of Eddy Diffusivity Variation on the Atmospheric Diffusion Equation

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Abstract

The advection diffusion equation was solved analytically using separation of variables technique, considering first the wind speed and eddy diffusivity as constants; second as variables dependent on vertical height *z*. Comparison between predicted two models and observed concentration on Inshas, Cairo (Egypt) is done.

Keywords

Advection-Diffusion Equation, Separation of Variable Technique, Pollution, Concentrations

1. Introduction

Air pollutants released from various sources affect directly or indirectly man and his environment. Air pollutants emitted from different sources are transported dispersed or deposited my meteorological and topographical conditions. Dispersion of pollutants in the atmosphere is governed by the following dominant mechanisms [1], mean air flow that transports the pollutants downwind and turbulent velocity fluctuations that disperse the pollutants in all directions. Under moderate to strong winds, the continuously emitted pollutants from a cone-shaped plume in the downwind direction of the source. In this case, advection in the mean wind direction dominates over diffusion and dispersion in the crosswind and vertical directions is assumed to be non-Gaussian. Along-wind diffusion is particularly important near the leading edge of the plume, where uncontaminated fluid from upwind mixes with the mass initially released [2].

Analytical solutions of the advection-diffusion equation are usually obtained just for stationary conditions and by making strong assumptions about the eddy diffusivity coefficients (K) and wind speed profiles (U). They are assumed as constant throughout the whole Atmospheric Boundary Layer (ABL) or follow a power law [3]-[6]. Moreira *et al.* presented a solution of the advection-diffusion equation based on the Laplace transform considering the ABL as a multilayer system [7]. Number of dispersion regulatory models includes improved dispersion algorithms in terms of fundamental scaling parameters [8]-[11]. Gryning *et al.* suggested a modeling approach composed by individual models [12]; each one based the specific turbulent structure of the regimes in the ABL, following [13]. The models give the crosswind-integrated concentrations at the ground, for non-buoyant releases from a continuous point source. They are limited to horizontally homogeneous conditions and travel distances less than 10 km.

Palazzi *et al.* have proposed a simple model for studying the diffusion of substances emitted in steady-state releases of short duration assuming the presence of an infinite mixing layer [14]. The Gaussian models, which are the best known and most widely used, are based on a solution of the two-dimensional advection equation where both the wind and exchange coefficients are assumed to be constant. The Gaussian model solution is forced to represent an inhomogeneous atmosphere through empirical dispersion parameters [15].

In this study, we have formulated a mathematical model for dispersion of air pollutants in moderated winds by taking into account the diffusion in vertical height direction and advection along the mean wind. The eddy diffusivity and wind speed are assumed to be constant. An analytical solution has been obtained for the resulting advection-diffusion equation with the physically relevant boundary conditions. The moderate data collected during the convective conditions. Nine experiments were conducted at Inshas site, Cairo-Egypt [16], which used to investigate the analytical solution.

2. Mathematical Treatment

The dispersion of pollutants in the atmosphere is governed by the basic atmospheric diffusion equation. Under the assumption of incompressible flow, atmospheric diffusion equation based on the Gradient transport theory can be written in the rectangular coordinate system as:

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

where *C* is the mean concentration of a pollutant (Bq/m³), (μ g/m³) and (ppm); *S* is the source term, respectively; (*u*, *v*, *w*) and (k_x , k_y , k_z) are the components of wind and diffusivity vectors in *x*, *y* and *z* directions, respectively, in an Eulerian frame of reference.

The following assumptions are made in order to simplify Equation (1):

1) Steady-state conditions are considered, *i.e.* $\partial C/\partial t = 0$.

2) As the vertical velocity is much smaller than the horizontal one in x-direction, the term $w(\partial C/\partial z)$ is neglected.

3) x-axis is oriented in the direction of mean wind u = U and U much greater than the wind speed v in y-direction the term $v(\partial C/\partial y)$ is neglected).

4) Source (physical/chemical) pollutants are ignored so that S = 0.

With the above assumptions, Equation (1) reduces to:

$$U\frac{\partial C}{\partial x} = \frac{\partial}{\partial x} \left(K_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial C}{\partial z} \right).$$
(2)

The advection term in x direction is larger than the diffusion in x direction then we will neglect the diffusion term in x direction,

$$U\frac{\partial C}{\partial x} = \frac{\partial}{\partial y} \left(K_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial C}{\partial z} \right).$$
(3)

Equation (3) is solved together with the following boundary conditions.

• The is assumed to be a perfectly total absorption *i.e.*,

$$\frac{\partial C(x,z)}{\partial z} = 0 \quad \text{at} \quad z = 0, z = h.$$
(4)

• The pollutant is totally penetrate through the top of the inversion/mixed layer located at height h,

i.e.

$$C(x, y, z) = 0 \quad \text{at} \quad z = h. \tag{5}$$

• A continuous point source with strength Q is assumed to be located at the point $(0, y_s, z_s)$, *i.e.*

$$UC = Q\delta(z - z_s) \text{ as } x = 0 \tag{6}$$

where $\delta(\cdots)$ is Dirac's delta function.

• Far away from the source, the concentration decreases to zero, *i.e.*

$$C \to 0 \text{ as } xy, z \to \infty.$$
 (7)

2.1. Variable Eddy Diffusivity and Wind Speed

Here we will use Equation (3), considering the wind speed U as linear of z:

$$U = k_0 u_* z, \ z \neq 0 \text{ and } U = U_0 \text{ at } z = 0$$
(8)

and eddy diffusivity k_z is expressed as functions of power law of z as:

$$k_z = u_1 z^n \tag{9}$$

where k_o is Von-Karmen constant and u_* is the friction velocity. Where u_1 is turbulence intensity. Also after integrating Equation (3) with respect to y from $(-\infty \text{ to } \infty)$, Equation (2) becomes:

$$k_o u_* z \frac{\partial C_y}{\partial x} = \frac{\partial}{\partial z} \left(u_1 z^n \frac{\partial C_y}{\partial z} \right)$$
(10)

which is simply reads:

$$\frac{\partial C_y}{\partial x} = \frac{u_1}{k_o u_*} z^{n-1} \frac{\partial^2 C_y}{\partial z^2} + \frac{u_1 n}{k_o u_*} z^{n-2} \frac{\partial C_y}{\partial z}.$$
(11)

One can solve the two-dimensional partial differential Equation (11) analytically by using the separation of variables technique. We take the solution of Equation (11) of the form:

$$C_{y}(x,z) = X(x) \cdot Z(z).$$
⁽¹²⁾

Differentiating Equation (12) partially with respect to x and z and substituting in Equation (11), we get two ordinary differential equations in the variables X and Z as follows:

$$\frac{1}{X}\frac{\mathrm{d}X}{\mathrm{d}x} = -\lambda^2 \tag{13}$$

and

$$\frac{\alpha z^{n-1}}{Z}\frac{\mathrm{d}^2 Z}{\mathrm{d}z^2} + \frac{\beta z^{n-2}}{Z}\frac{\mathrm{d}Z}{\mathrm{d}z} = -\lambda^2 \tag{14}$$

where λ^2 is a constant, $\alpha = u_1/k_o u_*$ and $\beta = u_1 n/k_o u_*$. The general solution of Equation (13) is given by

The general solution of Equation (13) is given by

$$X(x) = \gamma e^{-\lambda^2 x} \tag{15}$$

where γ is a constant.

Equation (14) becomes:

$$z^{2} \frac{d^{2}Z}{dz^{2}} + nz \frac{dZ}{dz} + \frac{\lambda^{2}}{\alpha} z^{3-n} Z = 0.$$
 (16)

Equation (16) which simply reads:

$$z_*^2 \frac{\mathrm{d}^2 Z_*}{\mathrm{d} z_*^2} + z_* \frac{\mathrm{d} Z_*}{\mathrm{d} z_*} + \left[\eta^2 z_*^2 - \mu^2\right] Z_* = 0 \tag{17}$$

where $\eta^2 = 4\lambda^2 / \alpha (3-n)^2$, $\mu = 1 - n/3 - i$.

The solution of Equation (14) is obtained in different boundary conditions as follows:

Equation (10) along with the following boundary condition corresponding to Equation (4) and Equation (5):

$$Z = 0$$
 at $z = 0, h.$ (18)

On changing the dependent Z and independent z variables in Equation (16) by means of the substitutes:

$$Z = z_{*}^{\frac{1-n}{3-n}} Z_{*}$$

$$z_{*} = z^{\frac{3-n}{2}}$$
(19)

Equation (17) is a Bessel equation and has a solution [17]:

$$Z = z^{\frac{1-n}{2}} \left[A J_{\mu} \left(\eta z^{\frac{3-n}{2}} \right) + B J_{-\mu} \left(\eta z^{\frac{3-n}{2}} \right) \right]$$
(20)

where j_{μ} and $J_{-\mu}$ the Bessel functions of first kind of order μ and $-\mu$, respectively, A and B are constants, application of the boundary condition Equation (18) at z = 0 in Equation (20) yields B = 0 and condition z = h Equation (18) gives rise:

$$h^{\frac{1-n}{2}}J_{\mu}\left(\eta h^{\frac{3-n}{2}}\right) = 0.$$
(21)

Equation (21) this represents Storm-Liouville Eigen value problem which have the corresponding Eigen functions:

$$Z_{\alpha}(z) = z^{\frac{1-n}{2}} J_{\mu}\left(\eta_{\alpha} z^{\frac{3-n}{2}}\right) \alpha = 1, 2, 3, \cdots, \infty.$$

$$(22)$$

The general of Equation (10) is obtained by using Equation (15), Equation (21) and Equation (22) as:

$$C_{y}(x,z) = z^{\frac{1-n}{2}} \left[\sum_{\alpha=1}^{\infty} A_{\alpha} J_{\mu} \left(\eta_{\alpha} z^{\frac{3-n}{2}} \right) \exp\left(-\lambda^{2} x\right) \right]$$
(23)

where $A_{\alpha}\alpha = 1, 2, 3, \dots, \infty$ are the unknown coefficients. Equation (23) represent the concentration distribution C_{ν} through the Fourier-Bessel series [18] corresponding to a set of Eigen function Z_{α} .

Estimation of the coefficients A_{α} 's for crosswind integrated concentrations: The source at x = 0, Equation (6) gives:

$$k_o u_* z^{\frac{3-n}{2}} \left[\sum_{\alpha=1}^{\infty} A_\alpha J_\mu \left(\eta_\alpha z^{\frac{3-n}{2}} \right) \right] = Q_p \delta(z - z_s).$$
⁽²⁴⁾

To determine the values of A_{α} we use the orthogonally of Eigen functions series [18].

Multiplying Equation (24) by $z^{\frac{1-n}{2}} J_{\mu} \left(\eta_{\beta} z^{\frac{3-n}{2}} \right) \beta \ge 0$ and integrating according to z from 0 to h, we get:

$$A_{\beta} = \frac{2Q_{p}z_{s}^{\frac{1-n}{2}}}{k_{o}u_{*}h^{2}} * \frac{J_{\mu}\left(\eta_{\beta}z_{s}^{\frac{3-n}{2}}\right)}{J_{\mu+1}^{2}\left(\eta_{\beta}h^{\frac{3-n}{2}}\right)}\beta \geq 1.$$
(25)

Substituting A_{β} in Equation (23), the final solution is given as follows:

$$C_{y}(x,z) = Q_{p} \frac{2(zz_{s})^{\frac{1-n}{2}}}{k_{o}u_{*}h^{2}} \sum_{\alpha=1}^{\infty} \frac{J_{\mu}\left(\eta_{\alpha}z^{\frac{3-n}{2}}\right) J_{\mu}\left(\eta_{\alpha}z^{\frac{3-n}{2}}\right)}{J_{\mu+1}^{2}\left(\eta_{\beta}h^{\frac{3-n}{2}}\right)} \exp\left(-\lambda^{2}x\right).$$
(26)

In which $\eta_{\beta}h^{\frac{3-n}{2}}$ is given as:

$$J_{\mu}\left(\eta_{\beta}h^{\frac{3-n}{2}}\right) = 0.$$
⁽²⁷⁾

2.2. Eddy Diffusivity and Wind Speed as Constant

Here we will use Equation (3), considering the wind speed U and eddy diffusivity k_z as constant: Also after integrating Equation (3) with respect to y from $(-\infty \text{ to } \infty)$, Equation (2) becomes:

$$u\frac{\partial C_{y}}{\partial x} = k\frac{\partial^{2} C_{y}}{\partial z^{2}}$$
(28)

which is simply reads:

 $\frac{\partial C_y}{\partial x} = \frac{k}{u} \frac{\partial^2 C_y}{\partial z^2}.$ (29)

One can solve the two-dimensional partial differential Equation (29) analytically by using the separation of variables technique. We take the solution of Equation (29) of the form:

$$C_{y}(x,z) = F(x)G(z).$$
(30)

Differentiating (30) partially with respect to x and z and substituting in Equation (29), we get two ordinary differential equations in the variables F(x) and G(x) as follows:

$$\frac{1}{F(x)}\frac{\mathrm{d}F(x)}{\mathrm{d}x} = -\lambda^2 \tag{31}$$

and

$$\frac{k_z}{u}\frac{\mathrm{d}^2 G(z)}{\mathrm{d}z^2} = -\lambda^2 G(z)$$
(32)

where λ^2 is a constant.

The general solution of Equation (31) is given by

$$F(x) = \gamma e^{-\lambda^2 x} \tag{33}$$

where γ is a constant.

Equation (32) becomes:

$$\frac{k_z}{u}\frac{\mathrm{d}^2G(z)}{\mathrm{d}z^2} + \lambda^2G(z) = 0$$
(34)

which have solution

$$G(z) = A\cos(\lambda^2 z) + Bi\sin(\lambda^2 z) \text{ where } i^2 = -1$$
(35)

where A and B are constant.

Then from Equation (33) and Equation (35) the general solution

$$C(x,z) = e^{-\lambda^2 x} \left(A \cos\left(\lambda^2 z\right) + B i \sin\left(\lambda^2 z\right) \right).$$
(36)

By differentiate Equation (36) with respect to z and applying the boundary conditions we get:

$$\frac{\partial C(x,z)}{\partial z} = e^{-\lambda^2 x} \left(A\lambda^2 \sin\left(\lambda^2 z\right) + B\lambda^2 i \cos\left(\lambda^2 z\right) \right). \tag{37}$$

Appling the boundary condition Equation (4) on Equation (37) which gives B = 0 and Equation (36) becomes:

$$C(x,z) = A\cos(\lambda^2 z)e^{-\lambda^2 x}.$$
(38)

Again apply the boundary condition Equation (6) leads to

$$A = \frac{Q}{uz_s} \sec\left(\lambda^2 z_s\right). \tag{39}$$

Substituting A in Equation (38), the final solution is given as follows:

$$C(x,z) = \frac{Q}{uz_s} e^{-\lambda^2 x} \cos(\lambda^2 z) \sec(\lambda^2 z_s).$$
(40)

In the Previous section we used the wind speed and eddy diffusivity as functions in the vertical height z, and we had the solution Equation (26). Now we have two forms of the solutions Equation (26) and Equation (40).

3. Applications

3.1. Source Data

The diffusion data for the estimating were gathered during ¹³⁵I isotope tracer nine experiments in moderate wind with unstable conditions at Inshas, Cairo. During each run, the tracer was released from source has height 43 m for twenty four hours working, where the air samples were collected during half hour at a height 0.7 m.

We collected air samples from 92 m to 184 m around the source in AEA, Egypt. The study area is at, dominated by sand soil with poor vegetation cover. The air samples collected were analyzed in Radiation Protection Department, NRC, AEA, Cairo, Egypt using a high volume air sampler with 220 V = 50 Hz bias [10]. Meteorological data have been provided by the measurements done at 10 and 60 m. **Table 1** gives the data information

Table 1. Meteorological data of	the nine convectiv	ve test runs at Inshas s	site in March and May 2006.

Run No.	Working hours	Release rate (Bq)	Wind speed $(\mathbf{m} \cdot \mathbf{s}^{-1})$	Wind direction (deg)	$W_* (\mathrm{m} \cdot \mathrm{s}^{-1})$	$Z_i(\mathbf{m})$	P-G stability class
1	48	1028571	4	301.1	2.27	600.85	А
2	49	1050000	4	278.7	3.05	801.13	А
3	1.5	42857.14	6	190.2	1.61	973	В
4	22	471428.6	4	197.9	1.23	888	С
5	23	492857.1	4	181.5	0.958	921	А
6	24	514285.7	4	347.3	1.3	443	D
7	28	1007143	4	330.8	1.51	1271	С
8	48.7	1043571	4	187.6	1.64	1842	С
9	48.25	1033929	4	141.7	2.1	1642	А

about the diffusion tests and the wind vectors. In addition, it contains values of vertical velocity scale (w_*) and mixing height (z_i). The data from these nine unstable test runs have been utilized for the following analysis.

Table 1 gives information about the diffusion tests and the wind vectors. In addition, it contains values of the vertical velocity scale (w_*).

3.2. Model Parameters

For the concentration computations, we require the knowledge of wind speed, wind direction, source strength, the dispersion parameters, mixing height and the vertical scale velocity. Wind speeds are greater than 3 m/s most of the time even at 10 m level. Further the variation wind direction with time is also visible. The analytical expressions depend upon downwind distance, vertical distance and atmospheric stability. The atmospheric stability has been calculated from Monin-Obukhov length scale (1/L) [19] based on friction velocity, temperature, and surface heat flux.

4. Results and Discussion

The concentration is computed using data collected at vertical distance of a 30 m multi-level micrometeorological tower. In all a test runs were conducted for the purpose of computation. The concentration at a receptor can be computed in the following way:

Applying formula Equation (26) which contains the wind sped and eddy diffusivity as variable and Equation (40) which contains the wind sped and eddy diffusivity as constant at y = 0.0 for half hourly averaging.

Table 2 contains the observed concentrations Bq/m³ and proposed concentrations in bounded and unbounded cases.

As an illustration, results computed from these approaches are shown in **Table 2**, for nine typical tests conducted at Inshas site, Cairo-Egypt [16]. This table shows that the predicted concentrations for ¹³⁵I using Equation (26) is very near to the observed concentration more than the predicted concentrations using Equation (40), because the eddy diffusivity and the wind speed were used as constants, on the other hand the eddy diffusivity and the wind speed had been used as functions in vertical height *z*, in Equation (26).

Figure 1 shows the variation of predicted and observed concentration of 135 I with the downwind distance. One gets good agreement between observed and predicted concentration Equation (26) more than predicted concentration Equation (40).

Figure 2 shows that the predicted concentrations which are estimated from Equation (26) and Equation (40) are a factor of two with the observed concentration.

Test	Downwind distance (m)	Vertical distance (m)	Observed conc. (Bq/m ³)	Predicted conc. Equation (40) (Bq/m ³)	Predicted conc. Equation (26) (Bq/m ³)
1	100	5	0.025	0.032	0.051
2	98	10	0.037	0.033	0.031
3	115	5	0.091	0.090	0.070
4	135	5	0.197	0.148	0.160
5	99	2	0.272	0.155	0.234
6	184	11	0.188	0.162	0.138
7	165	12	0.447	0.032	0.339
8	134	7.5	0.123	0.033	0.107
9	96	5.0	0.032	0.032	0.034

Table 2. Obse	rved and pre	edicted concentrat	tions for run	9 experiments.
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A. A. Marrouf et al.

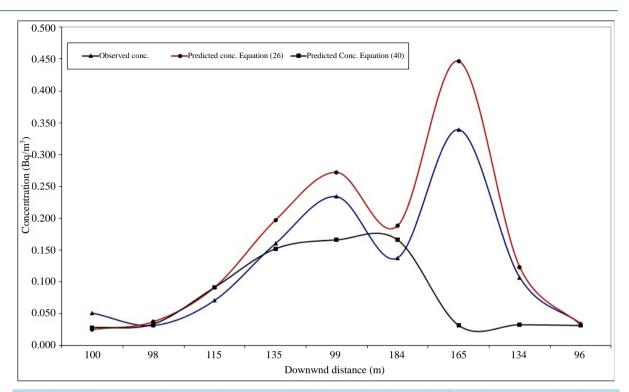


Figure 1. Maximum computed concentrations compared with observed maximum value for each test run Equation (26) and Equation (40).

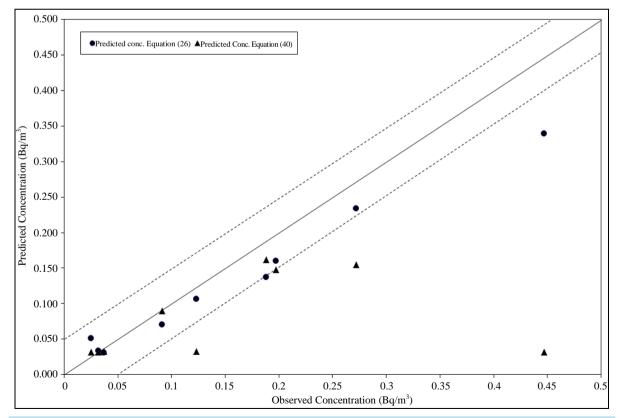


Figure 2. Diagram of predicted model for Equation (26) and Equation (40) with corresponding observation. Solid lines indicate one to one and dashed lines a factor of two.

5. Statistical Method

Now, the statistical method is presented and comparison among analytical, statically and observed results will be offered [20]. The following standard statistical performance measures that characterize the agreement between prediction ($C_p = C_{pred}$) and observations ($C_o = C_{obs}$):

1) Normalized mean square error (NMSE): It is an estimator of the overall deviations between predicted and observed concentrations. Smaller values of NMSE indicate a better model performance. It is defined as:

NMSE =
$$\frac{\left(C_o - C_p\right)^2}{\overline{C}_o \overline{C}_p}$$

2) Fractional bias (FB): It provides information on the tendency of the model to overestimate or underestimate the observed concentrations. The values of FB lie between -2 and +2 and it has a value of zero for an ideal model. It is expressed as:

$$\mathrm{FB} = \frac{\left(\overline{C}_o - \overline{C}_p\right)}{0.5\left(\overline{C}_o + \overline{C}_p\right)}$$

3) Correlation coefficient (R): It describes the degree of association between predicted and observed concentrations and is given by:

$$R = \frac{\left(C_o - \overline{C}_o\right)\left(C_p - \overline{C}_p\right)}{\sigma_o \sigma_p}.$$

4) Fraction within a factor of two (FAC2) is defined as:

FAC2 = fraction of the data for which

$$0.5 \leq \left(C_p / C_o \right) \leq 2$$

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 (N·m). A perfect model would have the following idealized performance: NMSE = FB = 0 and COR = FAC2 = 1.0.

From the statistical method of **Table 3**, we find that the predicted concentrations Equation (26) and Equation (40) for ¹³⁵I lies inside factor of 2 with observed data. Regarding to NMSE, FB and COR the predicted concentrations Equation (26) for ¹³⁵I is better with observed data more than predicted concentrations Equation (40), this is because in model of Equation (26) the wind speed and eddy diffusivity were used as functions in the vertical height *z*, contrast that Equation (40) the wind speed and eddy diffusivity were used as constant.

Table 3. Comparison between averages predicted isotopes for ¹³⁵ I and observed concentrations.					
Statistical functions	¹³⁵ I				
Statistical functions	NMSE	FB	COR	FAC2	
Predicated concentrations Equation (40)	1.75	0.65	0.29	0.74	
Predicated concentrations Equation (26)	0.10	0.19	0.99	0.4	

6. Conclusions

In this paper, we have formulated a mathematical model for dispersion of air pollutants in moderated winds. The diffusion in vertical height direction and advection along the mean wind are taking into account. The eddy diffusivity and the wind speed are assumed to be constant times and variable times. The analytical model is compared with data collected from nine experiments conducted at Inshas, Cairo (Egypt). One gets the predicted concentration Equation (40) that is in poor agreement with the corresponding observation in contrast Equation (26) that gives good agreement with the corresponding observation. Because the eddy diffusivity and the wind speed were used as constants (Equation (40)). On the other hand, the eddy diffusivity and the wind speed had been

used as functions in vertical height "*z*", in Equation (26).

Statistical method also shows that wind speed and eddy diffusivity are taken as a variable better than as a constant.

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