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The Concentration of Pollutants with Deposition under Different Atmospheric Stabilities

Khaled S. M. Essa, Soad M. Etman, Maha S. El-Otaify, *Ahmed M. Mosallem, H. M. Taha and [1]Ayman A. Khalifa

Department of Mathematics and Theoretical Physics, Nuclear Research Centre, Atomic Energy Authority, Cairo, Egypt

[1]Beni-Suef University, Department of Physics

**ahmedmetwally77@hotmail.com*

ABSTRACT

The dispersion of pollutants from a point source is analytically investigated taking into consideration the vertical variation of both wind speed and eddy diffusivity. A power-law profile was used to describe the variation of wind speed and vertical eddy diffusivity with height z above ground surface. The dry deposition of the diffusing particles at the ground surface is taken into account through the boundary conditions. The concentration of pollutants was derived assuming that the vertical diffusion is limited by an elevated impenetrable inversion layer located at the top of the boundary layer of height h. Also the decay distance of a pollutant along the wind direction was derived. The resulting analytical solution have been applied on two study cases namely, the emission from the Research Reactor at Inshas in unstable conditions and Hanford diffusion experiment in stable conditions. Comparisons between predicted and observed concentrations reveal a good agreement between them in the considered cases. The results are discussed and presented in illustrative figures.

Key words: Power law of wind speed and eddy diffusivity, decay distance of a polutant, Inshas and Hanford experiment

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INTRODUCTION

The diffusion from a point source in an urban atmosphere is studied by Essa and El-Otaify [1]. The effect of ground level absorption on the dispersion of pollutant has been studied analytically by Heines and Peters [2]. Bennett [3] introduced a physical model for the dry deposition of pollutants to a rough surface [1, 4-7].

Chrysikopoulos et al. [8] and Lin and Hildemann [9] derived the exact solutions of the advection-diffusion equation with dry deposition on the ground surface and for power law profiles of the vertical eddy diffusivity and wind speed in the unbounded atmosphere (infinite mixing/inversion layer) for the ground level area and point sources, respectively. However, an assumption of infinite unbounded ABL in derivation of these solutions is not physically realistic because of the formation of finite inversion/mixing layer in lower atmosphere that restrict the vertical pollutant diffusion. The surface based inversion in stable conditions influences most of the atmospheric.

Recently, Tirabassi et al. [10] and Kumar and Sharan [11] derived the solutions of the two-dimensional advection-diffusion equation by considering the deposition on the ground surface. However, the mathematical techniques to solve the advection-diffusion equation in Tirabassi et al. [10] and Kumar and Sharan [11], and also in other numerical or analytical solutions are required to verify with an exact solution of this equation.

In this paper an analytical treatment of the diffusion equation is presented under the boundary conditions which include the deposition of pollutants on the ground surface. The power-law profile was used to describe the variation of wind speed and vertical eddy diffusivity with height z above ground surface**.** The vertical diffusion is assumed to be limited by an elevated inversion layer, which tends to reflect back the air pollutants hitting the inversion base. The resulting analytical formulae have been applied on a case study namely, the emission from the Research Reactor at Inshas in unstable conditions and Hanford diffusion experiment in stable conditions. Statistical measures were used to evaluate the performance of the derived solution. The values of these measures show a good agreement between the observed and predicted concentrations. The results are discussed and presented in illustrative figures.

MATHEMATICAL DESCRIPTION

The diffusion equation in the steady state which describes the dispersion of pollutants in a turbulent atmospheric boundary layer is given as [12]:

$$u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}+\omega\frac{\partial C}{\partial z}=\frac{\partial}{\partial x}\left(k_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(k_z\frac{\partial C}{\partial z}\right)+R+S \quad (1)$$

where $C=C(x,y,z)$ is the mean contaminant concentration (g/m ^{3}), u,v,ω,k_x,k_y and k_z are the components of wind velocity (m /s) and eddy diffusivity coefficient (m^2 /s) along the x, y, and z directions, respectively, S and R are the source and removal terms.

The following assumptions are used to simplify Eq. (1):

1- The mean wind velocity is along the x-axis, i.e. $v=\omega=0$.
2- The diffusion in the direction of the mean wind is neglected compared to the advection in that direction.
3- The source and removal terms are ignored so that, S=0 and R=0.

Therefore Eq. (1) reduced to:

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

The solution of Eq. (3) can be obtained as follows:

1- Integrating Eq. (3) with respect to y from $-\infty$ to ∞, leads to

$$u\frac{\partial C_y}{\partial x}=\frac{\partial}{\partial z}\left(k_z\frac{\partial C_y}{\partial z}\right) \quad (3)$$

Where,

$$C_y(x,z)=\int_{-\infty}^{\infty}C(x,y,z)\,dy \quad (4)$$

is the crosswind integrated concentration.

2- Assuming the concentration distribution of pollutants in the crosswind direction is Gaussian [13] therefore, the three dimensional solution of Eq. (2) can be written as:

$$C(x,y,z)=C_y(x,z)\frac{1}{\sqrt{2\pi}\ \sigma_y}\ e^{-(y^2/2\sigma_y^2)} \quad (5)$$

where, σ_y is the lateral dispersion parameter (m).

A power-law profile is used to describe the variation of wind speed and vertical eddy diffusivity with height z in the atmospheric boundary layer as:

$$u(z)=\alpha z^p,\ \alpha=u_r z_r^{-p} \quad (6)$$

$$\mathrm{k(z)}=\mathrm{k_o}+\gamma\,\mathrm{z^n},\quad \gamma=\mathrm{k_r z_r^{-n}} \quad (7)$$

where p and n are the power-law exponent of wind speed and eddy diffusivity respectively, u_r and k_r are the wind speed and the eddy diffusivity at the reference height z_r respectively. The exponents p and n are functions of the atmospheric stability and nature of underlying surface.

Equation (3) is solved under the following boundary conditions:

$$C_y(x,z)=0 \text{ at } z=h \quad (8a)$$

$$k_z\frac{\partial C_y(x,z)}{\partial z}=0 \text{ at } z=h \quad (8b)$$

$$k_z\frac{\partial C_y(x,z)}{\partial z}=v_d C_y(x,z) \quad \text{at } z=0 \quad (8c)$$

$$Q=\int_0^{x_d}\int_0^h u(z)C_y(x,z)\,dz\,dx \quad (8d)$$

Notice that $k_z(z=0)=k_o$. The diffusion coefficient should be non-zero at the ground surface for vertical diffusion to be possible.

where Q is the emission rate, h is the mixing height, v_d is the deposition velocity of a pollutant and x_d is the decay distance of a pollutant radioactive or industrial..

Assuming the solution of Eq. (3) has the form [14]:

$$C_y(x,z)=F(x)\left(1-\frac{z}{h}\right)^2 \quad (9)$$

Integrating Eq. (3) with respect to "z" from 0 to h and applying the boundary conditions Eqs. (8a-8c), yields:

$$\frac{d}{dx}\int_0^h uC_y(x,z)dz=-v_d C_y(x,0) \quad (10)$$

Substituting by Eqs. (6 and 9) in Eq. (10) leads to:

$$\alpha\frac{dF(x)}{dx}\int_0^h z^p\left(1-\frac{z}{h}\right)^2 dz=-v_d F(x) \quad (11)$$

Let :

$$N=\int_0^h z^p\left(1-\frac{z}{h}\right)^2 dz=\frac{2h^{p+1}}{(p+1)(p+2)(p+3)} \quad (12)$$

Therefore, Eq.(11) takes the form:

$$\frac{dF}{dx} = -\frac{v_d}{\alpha N} F(x) \quad (13)$$

and has the following solution:

$$F(x) = F_0 e^{-\frac{v_d}{\alpha N}x} = F_0 e^{-\frac{x}{x_d}} \quad (14)$$

where F_0 is a constant of integration and

$$x_d = \frac{\alpha N}{v_d} \quad (15)$$

is called the decay distance of airborne pollutant radioactive or industrial. The concentration formula Eq. (9) can be written as:

$$C_y(x,z) = F_0 e^{-\frac{x}{x_d}} \left(1 - \frac{z}{h}\right)^2 \quad (16)$$

To determine F_0 substitute by Eq. (16) in the boundary condition Eq.(8d) yields:

$$Q = \alpha F_0 \int_0^{x_d} e^{-\frac{x}{x_d}} \int_0^h z^p \left(1 - \frac{z}{h}\right)^2 dz dx$$

$$= \alpha F_0 \int_0^{x_d} e^{-\frac{x}{x_d}} N dx$$

$$= x_d^2 v_d F_0 \left(1 - \frac{1}{e}\right) \quad (17)$$

Then,

$$F_0 = \frac{Qe}{x_d^2 v_d (e-1)} \quad (18)$$

Therefore, the crosswind integrated concentration takes the form:

$$C_y(x,z) = \frac{Qe}{x_d^2 v_d (e-1)} e^{-\frac{x}{x_d}} \left(1 - \frac{z}{h}\right)^2 \quad (19)$$

And Eq. (5) which is the general solution of Eq. (2) can be written as:

$$C(x,y,z) = \frac{Qe}{\sqrt{2\pi}\sigma_y x_d^2 v_d (e-1)} e^{-\left[\frac{y^2}{2\sigma_y^2} + \frac{x}{x_d}\right]} \left(1 - \frac{z}{h}\right)^2 \quad (20)$$

RESULTS AND DISCUSSION

In this work we present an analytical solution of the three dimensional advection-diffusion equation taking into account the dry deposition of the pollutants at ground surface. The derived concentration formula Eq.(20) was evaluated against the data of I-135 obtained from Inshas experiment. Also, the formula of the crosswind integrated concentration, Eq.(19) was evaluated against the data ofthe depositing tracer zinc sulfide (ZnS) obtained from Hanford diffusion experiment.

1- Inshas dispersion experiments in unstable conditions

The data used to calculate the concentration of I-135 isotope was obtained from dispersion experiments conducted in unstable conditions to collect air samples around the Research Reactor at Inshas. The samples were collected at a height of 0.7m above ground. The emissions were released from a stack of height 43m. The Reactor site was flat and dominated by sandy soil with a poor vegetation cover with a roughness length of0.6cm. The deposition velocity of Iodine v_d =0.01m/s. The measured concentration of I-135 isotope and the meteorological data during the experiments are taken from Essa & El-Otaify [1] and presented in Table (1). The values of power-law exponent p and n of wind speed and eddy diffusivity as a function of air stability are taken from Hanna et al. [15] and presented in Table (2). The crosswind dispersion parameter σ_y was calculated using Briggs formula [16] in urban area, see Table (3). The predicted concentrations by Eq. (20) below the plume center line are presented in Table (1). A comparison between predicted and observed concentrations of I-135 in unstable condition at Inshas are shown in Figs. (1 and 2).

2-Hanford diffusion experiment in stable conditions

The diffusion experiment was conducted at Hanford, south eastern Washington (46°34′N, 119°36′W) USA during May-Jun, 1983 on flat terrain with a roughness length of 3cm. Two tracers, one depositing tracer zinc sulfide (ZnS) and one gaseous sulfur hexafluoride (SF_6) were released at height 2m above ground surface. Concentrations measured at five sampling arcs 100, 200, 800, 1600 and 3200 m downwind from the source during moderately stable to near-neutral conditions. The samples were collected on each arc at a height 1.5 m above ground surface. The deposition velocity v_d was evaluated only for the last three distances. The collected data during the field tests were tabulated as crosswind integrated concentrations. Detailed description of the experiment was supplied by Doran and Horst [17]. The meteorological data and the crosswind integrated concentration data normalized by emission rate Q during the field tests were taken from Doran and Horst [17] and presented in Table (4). The height of the mixing layer h, not presented in the Hanford dataset, wascalculated by the following formula [14, 18] for stable air:

$$h = 0.4\left(u_* \frac{L}{|f|}\right)^{1/2}, \qquad \text{for } h/L \text{ f } 0 \tag{21}$$

Where, f =2Ω sin Φ is the Coriolis parameter, Ω is the angular velocity of the Earth and Φ is the latitude. The values of the friction velocity u_* and the Monin- Obukhove length L for each run are presented in Table (4).

Table -1 Meteorological parameters and concentrations measured at Inshasin unstable condition and the corresponding values predicted by Eq. (20)

Run	*Stability class*	*h (m)*	*Wind Direction (deg)*	*U_{10}m (m/s)*	*Q (Bq)*	*Distance (m)*	*Observed C (Bq/m^3)*	*Predicted C (Bq/m^3)*
1	A	600.85	301.1	4	1028571	100	0.025	0.0156
2	A	801.13	278.7	4	1050000	98	0.037	0.03175
3	B	973	190.2	6	42857.14	115	0.091	0.04824
4	C	888	197.9	4	471428.6	135	0.197	0.23352
5	A	921	181.5	4	492857.1	99	0.272	0.19256
6	D	443	347.3	4	514285.7	184	0.188	0.13198
7	C	1271	330.8	4	1007143	165	0.447	0.4835
8	C	1842	187.6	4	1043571	134	0.123	0.09108
9	A	1642	141.7	4	1033929	96	0.032	0.02414

The predicted normalized crosswind integrated concentrations (C(x,z)/Q) by Eq.(19) are presented in Table (4). A comparison between the predicted and observed normalized crosswind integrated concentrations of ZnS in stable condition (Hanford experiment) are shown in Figs.(3 - 4).

Statistical measures were used to evaluate the performance of the new model, their values are presented in Table (5).

Table -2 Power-law exponent p and n of wind speed and eddy diffusivity as a function of air stability in urban area

	A	**B**	**C**	**D**	**E**	**F**
p	0.15	0.15	0.20	0.25	0.40	0.60
n	0.85	0.85	0.80	0.75	0.60	0.40

Table -3 Briggs formulas [16] for $\sigma_y(x)$ and $\sigma_z(x)$ in urban area

Stability classes	**σ_z(m)**	**σy (m)**
A	$0.24x\ (1+0.001x\ )^{1/2}$	$0.32x\ (1+0.0004x)^{-1/2}$
B	$0.24x\ (1+0.001x)^{1/2}$	$0.32x\ (1+0.0004x)^{-1/2}$
C	$0.20x$	$0.32x\ (1+0.0004x)^{-1/2}$
D	$0.14x\ (1+0.0003x)^{-1/2}$	$0.16x\ (1+0.0004x)^{-1/2}$
E	$0.08x\ (1+0.00015x)^{-1/2}$	$0.11x\ (1+0.0004x)^{-1/2}$
F	$0.08x(1+0.00015x)^{-1/2}$	$0.11x\ (1+0.0004x)^{-1/2}$

Table -4 Meteorological parameters and the crosswind integrated concentrations data normalized by QatHanford experiment in stable conditions and the corresponding values predicted by Eq. (19).

Date	**u_* (cm/s^{-1})**	**h (m)**	**u (m/s^{-1})**	**L (m)**	**$\bar{v}_d$ (cm/s^{-1})**	**Distance (m)**	**Observed C_y/Q (sm^{-2})**	**Predicted C_y/Q (sm^{-2})**
18/05/83	40	325	7.61	166	4.21	800	0.00224	0.00289
26/05/83	26	135	3.23	44	1.93		0.00747	0.00615
05/06/83	27	182	4.74	77	3.14		0.00306	0.00360
12/06/83	20	104	3.00	34	1.75		0.00804	0.00569
24/06/83	26	157	3.07	59	1.56		0.00525	0.00730
27/06/83	30	185	3.17	71	1.17		0.00723	0.00695
18/05/83	40	325	8.53	166	4.05	1600	0.000982	0.00073
26/05/83	26	135	3.59	44	1.80		0.00325	0.00318

05/06/83	27	182	5.40	77	3.02		0.00132	0.00135
12/06/83	20	104	3.39	34	1.62		0.00426	0.00367
24/06/83	26	157	3.24	59	1.47		0.00338	0.00189
27/06/83	30	185	3.80	71	1.15		0.00252	0.00284
18/05/83	40	325	9.43	166	3.65	3200	0.000586	0.00061
26/05/83	26	135	3.83	44	1.74		0.0023 1	0.00300
05/06/83	27	182	6.32	77	2.84		0.000662	0.00090
12/06/83	20	104	3.75	34	1.31		0.00314	0.00210
24/06/83	26	157	3.46	59	1.14		0.00292	0.00282
27/06/83	30	185	4.37	71	1.10		0.00125	0.00121

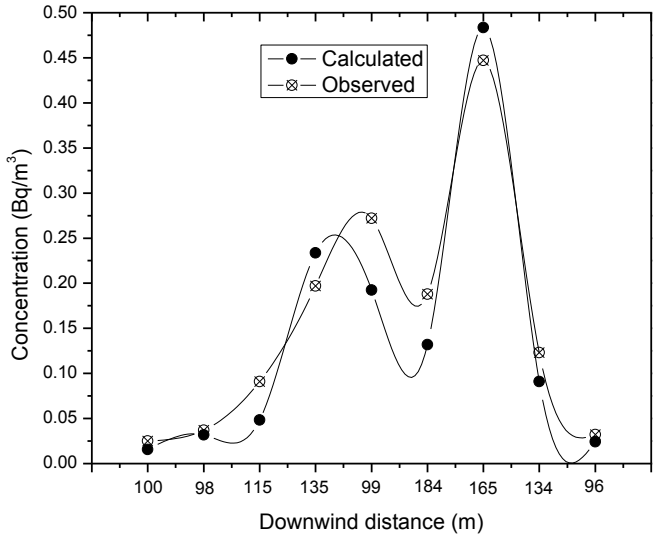

Fig. 1 Predicted and observed concentrations of ^{135}I via downwind distance in unstable condition at Inshas.

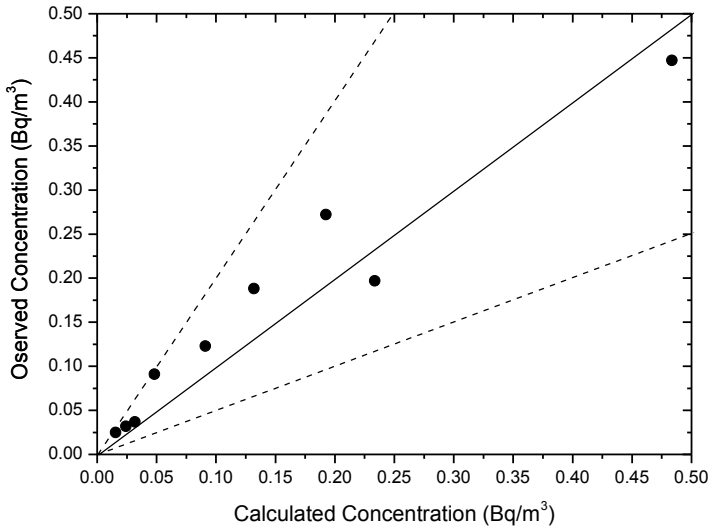

Fig. 2 Scatter diagram of observed and predicted concentrations of I-135 by the new model in unstable condition. at Inshas. The solid line and dashed lines indicate a one to one line and a factor of two respectively.

Figure (1) shows a good agreement between the observed concentrations of 135I and the corresponding values predicted by the derived formula Eq. (20). Fig.(2) illustrates that all values of the predicted concentrations by the new model Eq. (20) are inside a factor of two, so it presents a good agreement between the predicted and observed values.

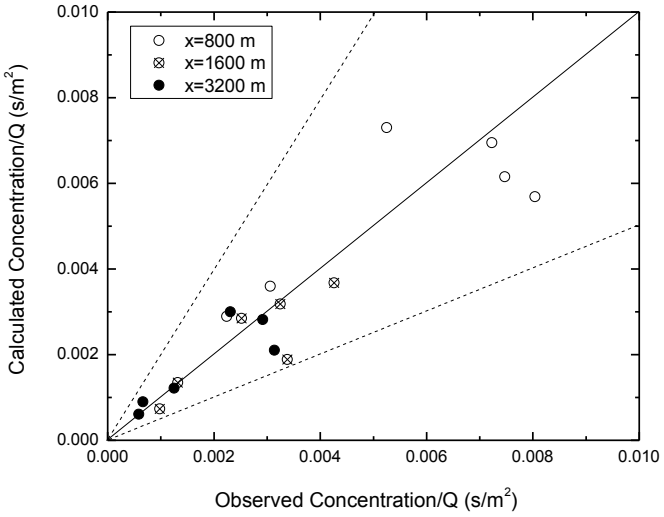

Fig. 3 Calculated normalized crosswind integrated concentrationsof ZnS againest the corrsponding observed values at Hanford experiment in stable condition. Dashed lines indicate a factor of two, solid line is the one-to-one line.

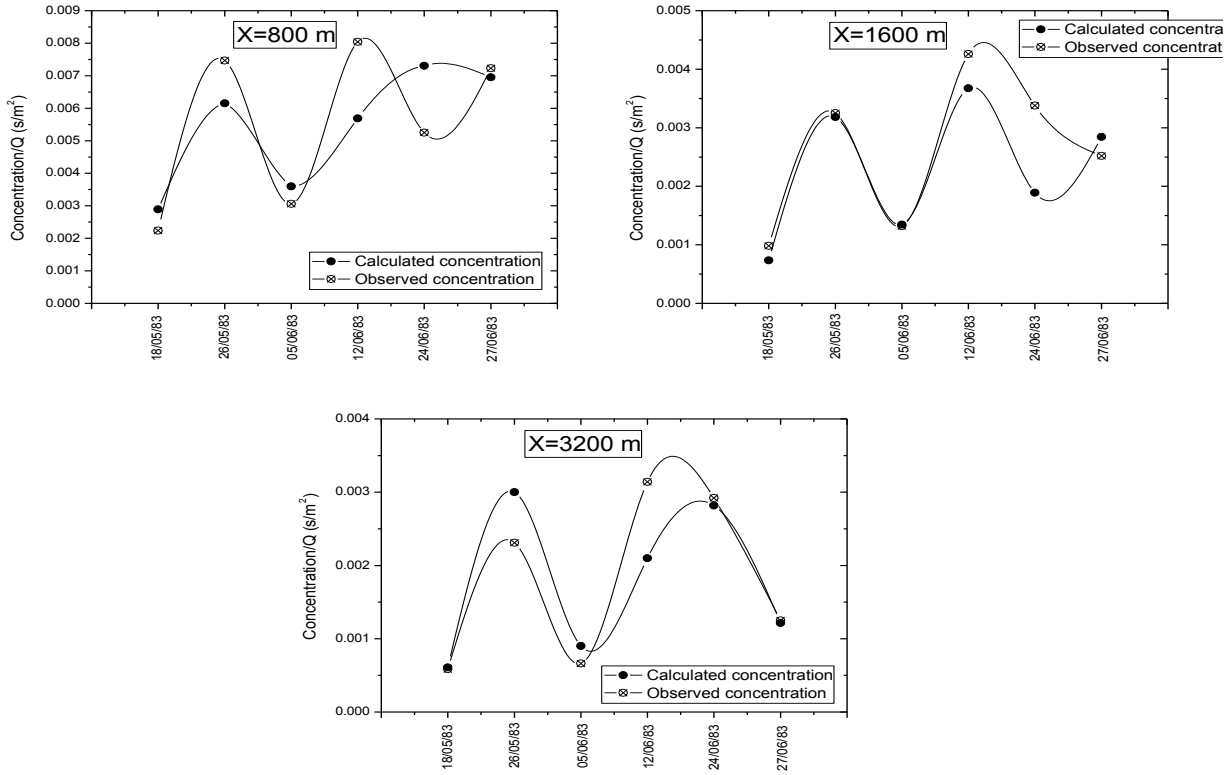

Fig. 4 Shows the variation of normalized observed and calculated crosswind integrated concentrations of ZnS at 800, 1600 and 3200m via date.

The scatter diagram (Fig.3) of the observed and predicted normalized crosswind integrated concentrations by the new model Eq. (19) reveals that all points lie within a factor of two, so it presents a good agreement between the predicted and observed values. Figures (4) show a reasonable agreement in most points between the calculated and observed normalized crosswind integrated concentrations.

MODEL EVALUATION STATISTICS

To evaluate the model accuracy we used the following statistical idiocies that characterize the agreement between the predicted and observed concentrations. These measures are discussed by Hanna [19] and defined as:

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

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

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

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

where σp and σo are the standard deviations of predicted (Cp=Cpred/Q) and observed (Co=Cobs/Q) concentration respectively. The overbar indicates the average value. The perfect model must have the following performances: NMSE = FB = 0 and COR= FAC2 = 1.0.

Table -5 Statistical evaluation of the present model against the Hanfordand Inshas experiments.

Experiments	NMSE	FB	COR	FAC2
Hanford at distance 800m	0.07	0.02	0.77	0.98
1600	0.08	0.14	0.86	0.87
3200	0.08	0.02	0.86	0.98
INSHAS	0.05	0.12	0.97	0.89

The values of the statistical indices Table (5) reveal a reasonable agreement between calculated and observed concentrations at Hanford experiment in stable conditions**,** and a good agreement at Inshas experiment during unstable **air**.

CONCLUSIONS

The concentration of pollutants under different atmospheric stabilities was found assuming that the vertical diffusion is limited by an elevated inversion layer. The decay distance of a pollutant along the wind direction for different atmospheric stabilities was derived. The resulting analytical formulae have been applied on two study Casses namely, Inshas and Hanford experiments. The Figs.(1- 4) and Tables (1 and 3) show a good agreement between the calculated and observed concentrations. Also, the values of the statistical indices in Table (5) reveal a reasonable agreement between calculated and observed concentrations at Hanford experiment**,** and a good agreement at Inshas experiment**.**

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