MAUSAM, **75**, 1 (January 2024), 237-244

MAUSAM

DOI : https://doi.org/10.54302/mausam.v75i1.5899
Homepage: https://mausamjournal.imd.gov.in/index.php/MAUSAM

UDC No. 502 : 551.553 : 519.16

Analytical concentration of pollutants with deposition using wind speed as power and logarithmic law

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(*Received 18 May 2022, Accepted 5 July 2023*)

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सार – **हवा में कणों की सांद्रता का गणितीय सूत्रीकरण विश्लेषणात्मक रूप से विसरण समीकरण को हल करके प्राप्त किया जाता है, जिसमें निम्नलिखित को ध्यान में रखा जाता है:** (*i*) **जमीन से ऊपर की ऊंचाई के साथ पवन वेग और प्रक्षुब्धत भंवर विसरणशीलता में भिन्नता।** (*ii*) **ऊर्ध्वाधर दिशा में प्रसार ऊंचाई** h **के साथ वायुमंडलीय सीमा परत** (ABL) **के शीर्ष द्वारा सीमित है।** (*iii*) **सतह परत पर सूखा जमाव होता है। प्रक्षुब्धस भंवर विसरणशीलता की भिन्नता को ऊँचाई** "z" **के शक्ति नियम के रूप में लिया जाता है, यह मानते हुए कि पवन वेग शक्ति नियम और ऊर्ध्वाधर दिशा में लघुगणकीय कानून प्रोफाइल का योग होता है। प्रदूषकों की क्षय दूरी ज्ञात की जाती है। वर्तमान समाधान की तुलना स्थानई स्थिरता में हैनफोर्ड प्रयोग के डेटासेट से की गई है। प्राप्तज परिणाम उदाहरणात्मक आंकड़ों में प्रस्तुत किए गए हैं और चर्चा की गई है।**

ABSTRACT. The mathematical formulation of the concentration of the particles in air is derived by solving analytically the diffusion equation taking into consideration: (*i*) the variation of wind velocity and turbulent eddy diffusivity with height above ground. (*ii*) diffusion in the vertical direction is limited by the top of Atmospheric Boundary Layer (ABL) with height h. (*iii*) there was dry deposition at the surface layer. The variation of turbulent eddy diffusivity is taken as a power law of height "z", considering the wind velocity is the sum of power law and the logarithmic law profiles in the vertical direction. The decay distance of pollutants, is derived. The present solution is compared against the dataset from theHanford experiment in stable stability. The results are presented and discussed in illustrative figures.

Key words – Power and the logarithmic law of wind speed, Vertical turbulent eddy diffusivity, Decay distance of pollutants, The Hanford experiment.

1. Introduction

The diffusionin an urban atmosphere from a point source was explained by Essa and El-Otaify (2006). The effect of ground level absorption on the dispersion of pollutant, had been studied analytically by Heines and Peters (1974). Bennett (1988), introduced a physical model for the dry deposition of pollutants to a rough surface.

The true solutions of the diffusion equation with dry deposition on the ground surface and power law profiles of the vertical turbulent eddy diffusivity and wind velocity in the unbounded atmosphere for the ground level area and point sources, was estimated by Essa *et al*., 2007; Vilhena *et al*., 2008; Moreira *et al*., 2009; Kumar and Sharan, (2010, 2012). Chrysikopoulos *et al*., (1992) and Lin and Hildemann (1997) respectively.

Recently, the solutions of the two-dimensional diffusion equation considering the deposition on the ground surface was evaluated by Tirabassi *et al*., (2008), Kumar and Sharan (2014). An advection-diffusion equation was solved in numerical or analytical solutions by Tirabassi *et al*., (2008), Kumar and Sharan (2014). Essa *et al*., (2020) derived the solution of an advection-diffusion equation in two dimensions with variable vertical turbulent eddy diffusivity and wind velocity (Table 1) using Hankel transform. Also, Essa *et al*., (2021) got the solution of advection-diffusion equation in three-dimensionsby Hankel transform.

In this research, the mathematical treatment of the diffusion equation is estimated considering the deposition of pollutants on the ground surface, taking wind velocity consists of the sum of the power and the logarithmic profiles and vertical turbulent eddy diffusivity is a

function of height z above surface layer. Considering the vertical diffusion is limited by an elevated inversion layer, the proposed analytical formulae have been used to compare with the Hanford experiment in stable condition. Statistical method explains the quality of the proposed solution.

2. Mathematical techniques

The dispersion of pollutants is described in ABL in the steady state by diffusion equation (Blackadar, 1997) as follows:

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

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

The assumptions are used to simplify Eqn. (1) as follows:

(*i*) The mean wind speed is in the *x*-axis, *i.e.*,$v=\omega=0$.

(*ii*) The diffusion of wind speed in *x*-direction is neglected compared to the advection term in a horizontal direction.

(*iii*) The source and removal terms are ignored, *i.e.*, S=0 and R=0.

Therefore, Eqn. (1) becomes:

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

Eqn. (2) is solved as follows:

2.1. Eqn. (2) is integrated from "*y*"equals -∞ to ∞ to get the crosswind integrated concentration as follows:

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

where,

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

TABLE 1

The values of p and n of wind velocity and turbulent eddy diffusivity

	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

2.2. The solution of Eqn. (2) in the three-dimension is as follows (Essa *et al*., 2016):

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

where, σ_y is the dispersion parameter in *y*-direction (m).

The vertical variation of wind speed is described as follows:

(*i*) *For Neutral Case*

$$u(z)=u_1\left(\frac{z}{z_r}\right)p+\frac{u_*}{k}1n\left(\frac{z+z_o}{z_o}\right) \quad (6a)$$

(*ii*) *For Stable Case*

$$u(z)=u_1\left(\frac{z}{z_r}\right)p+\frac{u_*}{k}1n\left(\frac{z+z_o}{z_o}+\frac{5.2z}{L}\right) \quad (6b)$$

(*iii*) *For Unstable Case*

$$u(z)=u_1\left(\frac{z}{z_r}\right)p+\frac{u_*}{k}\left\{\ln\left[\frac{\left[1+f(z)\right]^{\frac{1}{4}}-1}{\left[1+f(z)\right]^{\frac{1}{4}}+1}\right]+2\tan^{-1}\left[1+f(z)\right]^{\frac{1}{4}}+\ln\left[\frac{\left(1+\frac{16z_o}{L}\right)^{\frac{1}{4}}+1}{\left(1+\frac{16z_o}{L}\right)^{\frac{1}{4}}-1}\right]+2\tan^{-1}\left(1+\frac{16z_o}{L}\right)^{\frac{1}{4}}\right\} \quad (6c)$$

where, $f(z)=16(z+z_o)$, z_0 is the roughness length (m).

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

Notice that k_z (z =0) = k_o.

where, u_r and k_r are the wind velocity and the turbulent eddy diffusivity at reference height z_r (10m) respectively.

Eqn. (3) is estimated using the boundary conditions:

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

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

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

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

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

Let the solution of Eqn. (3) as follows (Essa *et al*., 2007):

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

Eqn. (3) is integrating with respect to "z" from 0 to h and applying Eqns. (8a-8c), yields:

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

Substituting from Eqns. (6 and 9) in Eqn. (10) leads to:

$$\frac{dF(x)}{dx}\int_0^h \left[az^p + \frac{u_*}{k}\ln\left(\frac{z+z_o}{z_o}\right)\right]\left(1-\frac{z}{h}\right)^2 dz = -v_d F(x) \tag{11}$$

where, $\alpha = \frac{u_1}{10^p}$, Let:

$$N_1 = \int_0^h \left[az^p + \frac{u_*}{k}\ln\left(\frac{z+z_o}{z_o}\right)\right]\left(1-\frac{z}{h}\right)^2 dz$$

$$= \frac{2\alpha h^{p+1}}{(p+1)(p+2)(p+3)} + \frac{u_* z_0^3}{3kh^2}\left(1+\frac{h}{z_o}\right)^3 \ln\left(1+\frac{h}{z_o}\right) - \frac{u_* z_o^2}{18kh}\left[6+\frac{15h}{z_o}+11\frac{h^2}{z_o^2}\right] \tag{12}$$

Therefore, Eqn. (11) takes form:

$$\frac{dF}{dx} = -\frac{v_d}{N_1}F(x) \tag{13}$$

and it has the following solution:

$$F(x) = F_0 e^{-\frac{vd_x}{N_1}} = F_0 e^{-\frac{x}{x_{dn}}} \tag{14}$$

where, the F_0 is a constant value and

$$X_{dn} = \frac{N_1}{v_d} \tag{15}$$

where, x_{dn} is the distance of decay pollutant radioactive. Then, Eqn. (9) can be written as follows:

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

Substituting from Eqn. (16) in Eqn. (8d) to get F_0

$$Q = F_0 \int_o^{x_d} e^{-\frac{x}{x_{dn}}} \int_0^h \left[\alpha z^p + \frac{u_*}{k}\ln\left(\frac{z+z_0}{z_0}\right)\right]\left(1-\frac{z}{h}\right)^2 dz dx$$

$$= F_0 \int_0^{x_d} e^{-\frac{x}{x_{dn}}} N_1 dx$$

$$= x_{dn}^2 v_d F_0 \left(1-\frac{1}{e}\right) \tag{17}$$

Then,

$$F_0 = \frac{Q_e}{x_{dn}^2 v_d (e-1)} \tag{18}$$

Therefore, integrated concentration in the crosswind takes the form in neutral conditions (Essa *et al*., 2007):

$$C_y(x,z) = \left[\frac{Q_e}{x_{dn}^2 v_d (e-1)} + \frac{Q}{0.63 x_{dn}^2 v_d}\right] e^{-\frac{x}{x_{dn}}}\left(1-\frac{z}{h}\right)^2 \tag{19}$$

$X_{dn} = \frac{N_1}{v_d}$, and

$$N_1 = \frac{2\alpha h^{p+1}}{(p+1)(p+2)(p+3)} + \frac{u_* z_o^3}{3kh^2}\left(1+\frac{h}{z_o}\right)^3 \ln\left(1+\frac{h}{z_o}\right) - \frac{u_* z_o^2}{18kh}\left[6+\frac{15h}{z_o}+11\frac{h^2}{z_o^2}\right]$$

Also, the C_y in stable conditions is in the form (Essa *et al*. 2007):

$$C_y(x,z) = \left[\frac{Qe}{x_d^2 v_d(e-1)} + \frac{Q}{0.63 V_d x_{ds}^2}\right] e^{-\frac{x}{x_{ds}}}\left(1-\frac{z}{h}\right)^2 \quad (20)$$

$$X_{ds} = \frac{M}{V_d} \text{ where, } M = N_1 - (5.2\ h^2/12L).$$

where, X_{ds} is the distance of decay pollutant, in stable condition.

Also, C_y is in unstable conditions as follows (Essa *et al*., 2007):

$$C_y(x,z) = \left[\frac{Qe}{x_{du}^2 v_d(e-1)} + \frac{Q}{0.63 v_d x_{du}^2}\right] e^{-\frac{x}{x_{du}}}\left(1-\frac{z}{h}\right)^2 \quad (21)$$

$$x_{du} = \frac{D}{v_d}$$

where, x_{du} is the distance of decay pollutant, in unstable condition and D is taken from (Essa *et al*., 2007).

Then, Eqn. (5) in neutral, stable and unstable conditions can be written [Eqns. (19 to 21)] as follows:

$$C(x,y,z) = C_y(x,z)\frac{1}{\sqrt{2\pi}\sigma_y} e^{-\left[\frac{y^2}{2\sigma_y^2}\right]} \quad (22)$$

where, C (x, y, z) is given by Eqns. (19 to 21) in neutral, stable and unstable conditions respectively.

McElroy and Pooler's (1968) diffusion experiment in St. Louis was used by Briggs (1973) to develop the formulas given in Table (2) as follows:

TABLE 2

Formulas recommended by Briggs (1973) for $\sigma_y(x)$ 10^2<x<10^4min urban area

A-B	$0.32x(1+0.0004x)^{-1/2}$
C	$0.22x(1+0.0004x)^{-1/2}$
D	$0.16x(1+0.0004x)^{-1/2}$
E-F	$0.11x(1+0.0004x)^{-1/2}$

where, A is extremely unstable, B is modularity unstable, C is slightly unstable, D is neutral condition and E , F are slightly and modularity stable.

3. Results and discussion

In this research, an analytical solution of the three-dimensional advection-diffusion equations taking into account the dry of the deposition pollutants at ground surface has been presented formula of C_y (x,z), Eqn. (20) is estimated against the data of the depositing zinc sulfide (ZnS) which obtained from the Hanford experiment in stable condition.

The experiment was made at the 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 zinc sulfide (ZnS) and one gaseous sulfur hexafluoride (SF_6) were released at height 2 m above the surface layer. Concentrations was 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 the ground surface. v_d is the deposition velocity was evaluated only for the last three distances. Detailed description of the experiment was supplied by Doran and Horst (1985). The meteorological data and the crosswind integrated concentration data normalized by emission rate Q during the field tests were taken from Doran and Horst (1985) and presented in Table (3). The height of the mixing layer, h, not presented in the Hanford dataset, was calculated by the following formula (Arya, 1999 and Essa *et al*., 2007) for stable air:

$$h = \left(u_* L/|f|\right)^{0.5}, \text{ for } h/L > 0 \quad (23)$$

where, f is the Coriolis parameter, u_* is the friction speed and L is the Monin- Obukhove length for each run are presented in Table (3).

Comparisons between the proposed concentrations C_y/Q by Eqn. (20) and observed concentrations of zincsulfide Cy/Q in stable condition (the Hanford experiment) are shown in Table (3) and Figs. 1&2.

TABLE 3

Meteorological and C_y normalized by Q at the Hanford experiment in stable conditions and the corresponding values of predicted (1) for power law, predicted (2) for the logarithmic law and predicted (3) for the sum of power and the Logarithmic laws Eqn. (20)

Date	$u_*(cm/s^{-1})$	L(m)	$\bar{v}_d(cm/s^{-1})$	Obs. $C_y/Q(sm^{-2})$	Pred. (1) $C_y/Q(sm^{-2})$	Pred. 2 $C_y/Q(sm^{-2})$	Pred. 3 $C_y/Q(sm^{-2})$
				800 m			
18/05/83	40	166	4.21	0.00224	0.00289	0.001356	0.004246
26/05/83	26	44	1.93	0.00747	0.00615	0.004103	0.010253
05/06/83	27	77	3.14	0.00306	0.00360	0.005302	0.008902
12/06/83	20	34	1.75	0.00804	0.00569	0.010682	0.016372
24/06/83	26	59	1.56	0.00525	0.00730	0.003153	0.010453
27/06/83	30	71	1.17	0.00723	0.00695	0.001318	0.008268
				1600 m			
18/05/83	40	166	4.05	0.000982	0.00073	0.001323	0.002053
26/05/83	26	44	1.80	0.00325	0.00318	0.003886	0.007066
05/06/83	27	77	3.02	0.00132	0.00135	0.005222	0.006572
12/06/83	20	34	1.62	0.00426	0.00367	0.010121	0.013791
24/06/83	26	59	1.47	0.00338	0.00189	0.003008	0.004898
27/06/83	30	71	1.15	0.00252	0.00284	0.001306	0.004146
				3200m			
18/05/83	40	166	3.65	0.000586	0.00061	0.00122	0.00183
26/05/83	26	44	1.74	0.0023 1	0.00300	0.003875	0.006875
05/06/83	27	77	2.84	0.000662	0.00090	0.005129	0.006029
12/06/83	20	34	1.31	0.00314	0.00210	0.008444	0.010544
24/06/83	26	59	1.14	0.00292	0.00282	0.002367	0.005187
27/06/83	30	71	1.10	0.00125	0.00121	0.001267	0.002477

TABLE 4

Statistical evaluation of the proposed model and the Hanford experiments

The Hanford Experiments	NMSE	FB	COR	FAC2
800m (power)	0.07	0.02	0.77	0.98
800 m (Logaritmic)	0.44	0.25	0.42	0.78
800m (sum)	0.44	-0.55	0.73	1.76
1600m (power)	0.08	0.14	0.86	0.87
1600 m (Logaritmic)	0.43	0.37	0.51	0.69
1600m (sum)	0.33	-0.44	0.80	1.56
3200m (power)	0.08	0.02	0.86	0.98
3200 m (Logaritmic)	0.20	-0.23	0.86	1.26
3200m (sum)	0.93	-0.77	0.91	2.24

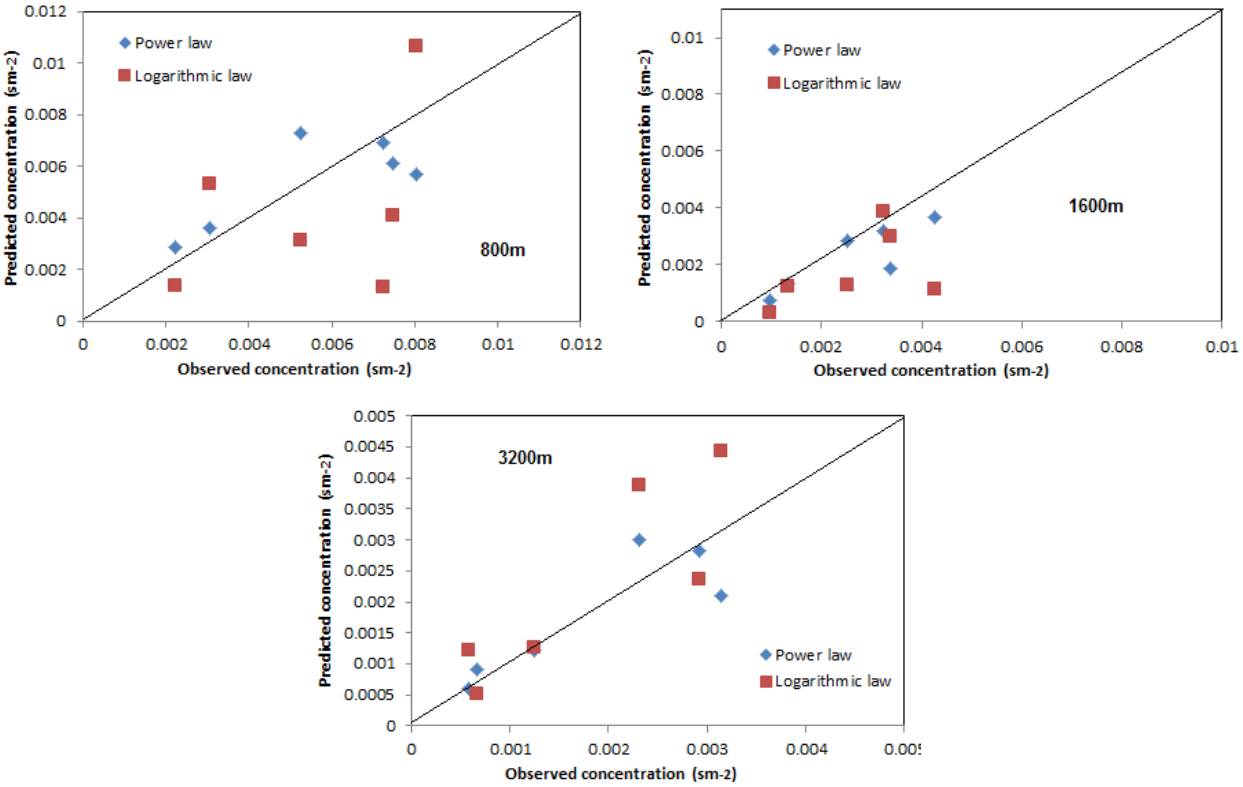

Fig. 1. Calculated C_y/Q concentrations of ZnS against the observed values at the Hanford experiment in stable condition at 800, 1600 and 3200m respectively

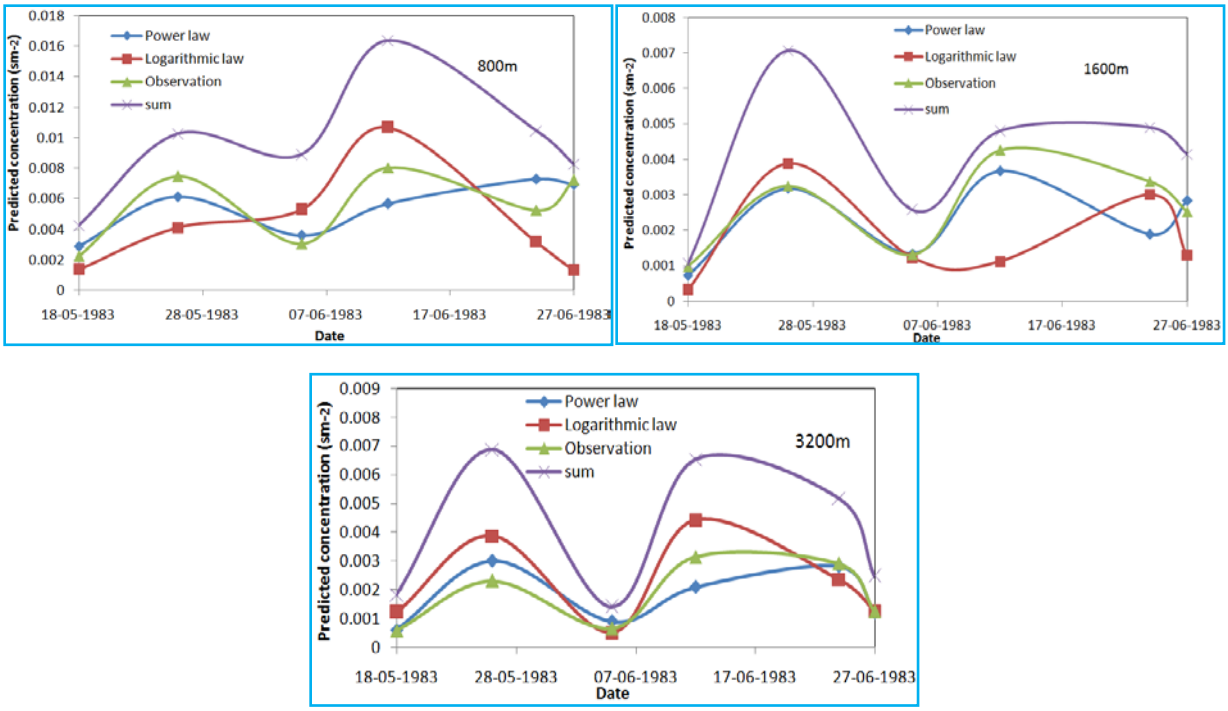

Fig. 2. Shows the variation of normalized observed and C_y/Q predicted concentrations of ZnS at 800, 1600 and 3200m *via* date

sulfide Cy/Q in stable condition (the Hanford experiment) are shown in Table (3) and Figs. 1&2.

Statistical methods are used to show the performance of the proposed model; in Table (4).

The observed and predicted concentrations C_y/Q with the new model of Eqn. (20) shows that all points lie within a factor of two as shown in Fig. 1, so that there is a good agreement between the proposed and observed values. Fig. 2 shows that a power law of the wind velocity is a good agreement in most points between the proposed and observed of C_y/Q concentrations than the logarithmic law of the wind velocity. Fig. 2 shows that the sum of the power and the logarithmic law of the wind velocity are greater than the observed concentrations.

4. Statistics techniques

To estimate the accuracy of the model, we used the following statistical methods to find that there is agreement between the proposed and observed concentrations as follows (Hanna, 1989).

$$\text{Fraction Bias (FB)} = \frac{\left(\overline{C}_o - \overline{C}_p\right)}{\left[0.5\left(\overline{C}_o + \overline{C}_p\right)\right]}$$

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

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

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

where, σ_p and σ_o are the standard deviations of proposed (C_p=C_{pred}/Q) and observed (C_o=C_{obs}/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 (4) shows that there is a good agreement between proposed and observed concentrations at the Hanford experiment in stable conditions, at 800, 1600 and 3200 m when using the wind velocity as power law than the logarithmic law. The proposed concentration data has achieved 94% from observed data when using the wind velocity as power law but almost 90% when using the wind velocity in the logarithmic law.

5. Conclusions

The concentration of pollutants under different atmospheric neutral, stable and unstable stabilities was found assuming that the vertical diffusion is limited by an elevated inversion layer. The distance of decay pollutant, along the wind direction for different atmospheric stabilities was derived. The wind velocity is the sum of the Logarithmic and power law. The proposed model is used to compare with the observed data from the Hanford experiments in stable conditions. One finds that there is a good agreement between the proposed and observed concentrations when the wind velocity is used as power law than the wind velocity is used as the logarithmic law as shown as in Figs. (1-2). Also, the values of the statistical indices shows that the proposed concentration data has achieved 94%from observed data when using the wind speed as power law but almost 90% when using the wind speed as logarithmic law as shown as in Table (4). The sum of the power and the logarithmic law of the wind velocity are greater than the observed concentrations.

Acknowledgement

The authors thank their God. Also, they thank the chief Editor of the journal and all members in my department.

Disclaimer : The contents and views expressed in this study are the views of the authors and do not necessarily reflect the views of the organizations they belong to.

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