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

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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 the Hanford 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 diffusion in 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-dimensions by 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:

\[
\frac{\partial C}{\partial t} + \frac{\partial}{\partial x} \left( \frac{
u}{k_x} \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{
u}{k_y} \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( \frac{\nu}{k_z} \frac{\partial C}{\partial z} \right) + \frac{\partial}{\partial z} \left( \frac{\partial C}{\partial x} \right) + R + S = 0
\]

(1)

where, \( C(x,y,z) \) is the pollutant concentration (g/m\(^3\)), \( u, v, \omega, k_x, k_y, \) 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, \( i.e., \nu=0=0 \).

(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:

\[
\frac{\partial C}{\partial t} + \frac{\partial}{\partial y} \left( \frac{k_y}{\nu} \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( \frac{k_z}{\nu} \frac{\partial C}{\partial z} \right) + \frac{\partial}{\partial z} \left( \frac{\partial C}{\partial x} \right) + R + S = 0
\]

(2)

Eqn. (2) is solved as follows:

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

\[
\frac{\partial C_y}{\partial x} = \frac{\partial}{\partial z} \left( \frac{k_z}{\nu} \frac{\partial C_y}{\partial z} \right)
\]

(3)

where,

\[
C_y(x,z) = \int_{-\infty}^{\infty} C(x,y,z) \, dy
\]

(4)

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

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

(5)

where, \( \sigma_y \) is the dispersion parameter in \( y \)-direction (m).

The vertical variation of wind speed is described as follows:

(i) For Neutral Case

\[
u(z) = u_1 \left( \frac{z}{z_r} \right) p + \frac{u_*}{k} \ln \left( \frac{z + z_o}{z_o} \right)
\]

(6a)

(ii) For Stable Case

\[
u(z) = u_1 \left( \frac{z}{z_r} \right) p + \frac{u_*}{k} \ln \left( \frac{z + z_o}{z_o} + \frac{5.2z}{L} \right)
\]

(6b)

(iii) For Unstable Case

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

(6c)

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

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

(7)

TABLE 1

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td>p</td>
<td>0.15</td>
<td>0.15</td>
<td>0.20</td>
<td>0.25</td>
<td>0.40</td>
<td>0.60</td>
</tr>
<tr>
<td>n</td>
<td>0.85</td>
<td>0.85</td>
<td>0.80</td>
<td>0.75</td>
<td>0.60</td>
<td>0.40</td>
</tr>
</tbody>
</table>

The values of \( p \) and \( n \) of wind velocity and turbulent eddy diffusivity.
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:

\[
C_y(x,z) = 0 \text{ at } z = h
\]  

(8a)

\[
k_z \frac{\partial C_y(x,z)}{\partial z} = 0 \text{ at } z = h
\]  

(8b)

\[
k_z \frac{\partial C_y(x,z)}{\partial z} = v_d C_y(x,z) \text{ at } z = 0
\]  

(8c)

\[
Q = \int_0^{z_r} \int_0^h u(z) C_y(x,z) dz dx
\]  

(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 decay pollutant radioactive or industrial.

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

\[
C_y(x,z) = F(x) \left(1 - \frac{z}{h}\right)^2
\]  

(9)

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

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

(10)

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

\[
\frac{dF}{dx} \int_0^h \left[ \alpha z^p + \frac{u_z}{k} \ln \left( \frac{z + z_0}{z_o} \right) \right] \left(1 - \frac{z}{h}\right)^2 dz = -v_d F(x)
\]  

(11)

where, \( \alpha = \frac{u_1}{10^p} \). Let:

\[
N_1 = \int_0^h \left[ \alpha z^p + \frac{u_z}{k} \ln \left( \frac{z + z_0}{z_o} \right) \right] \left(1 - \frac{z}{h}\right)^2 dz
\]  

(12)

Therefore, Eqn. (11) takes form:

\[
\frac{dF}{dx} = -\frac{v_d}{N_1} F(x)
\]  

(13)

and it has the following solution:

\[
F(x) = F_0 e^{\frac{-v_d}{N_1} \int_0^x \frac{dF}{dx} dx} = F_0 e^{-\frac{x}{x_d}}
\]  

(14)

where, the \( F_0 \) is a constant value and

\[
X_{dn} = \frac{N_1}{v_d}
\]  

(15)

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

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

(16)

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

\[
Q = F_0 \int_0^x e^{\frac{-x}{x_{dn}}} N_1 dx
\]  

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

= \( x_d^2 \nu_d F_0 \left(1 - \frac{1}{e}\right)
\]  

(17)

Then,

\[
F_0 = \frac{Q}{x_{dn} \nu_d (e - 1)}
\]  

(18)

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

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

(19)

\[
X_{dn} = \frac{N_1}{v_d}
\]  

and
\[ N_1 = \frac{2\alpha h^{p+1}}{(p+1)(p+2)(p+3)} + \frac{u_* z_0^3}{3kh^2} \left(1 + \frac{h}{z_0}\right)^3 \ln\left(1 + \frac{h}{z_0}\right) \]
\[ - \frac{u_* z_0^3}{18kh} \left[ 6 + 15h + 11h^2 \right] \]

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

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

(20)

\[ X_{ds} = \frac{M}{v_d} \]

where, \( M = N_1 - (5.2 \text{ h}^3/12L) \).

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):

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

(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:

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

(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>
<thead>
<tr>
<th>A-B</th>
<th>( 0.32x(1+0.0004x)^{1/2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>( 0.22x(1+0.0004x)^{1/2} )</td>
</tr>
<tr>
<td>D</td>
<td>( 0.16x(1+0.0004x)^{1/2} )</td>
</tr>
<tr>
<td>E-F</td>
<td>( 0.11x(1+0.0004x)^{1/2} )</td>
</tr>
</tbody>
</table>

TABLE 2
Formulas recommended by Briggs (1973)
for \( \sigma_x(x) \) 10^6<x<10^8 min urban area

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 \((\text{SF}_6)\) 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:

\[
h = \left( \frac{u_* L/|f|}{5.0} \right)^{0.5}, \text{ for } h/L > 0
\]

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

Meteorological and $C_v$ 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)

<table>
<thead>
<tr>
<th>Date</th>
<th>$u_\ast$ (cm/s$^{-1}$)</th>
<th>$L$ (m)</th>
<th>$v_d$ (cm/s$^{-1}$)</th>
<th>Obs. $C_v/Q$ (s m$^{-2}$)</th>
<th>Pred. (1) $C_v/Q$ (s m$^{-2}$)</th>
<th>Pred. 2 $C_v/Q$ (s m$^{-2}$)</th>
<th>Pred. 3 $C_v/Q$ (s m$^{-2}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>800 m</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>18/05/83</td>
<td>40</td>
<td>166</td>
<td>4.21</td>
<td>0.00224</td>
<td>0.00289</td>
<td>0.001356</td>
<td>0.004246</td>
</tr>
<tr>
<td>26/05/83</td>
<td>26</td>
<td>44</td>
<td>1.93</td>
<td>0.00747</td>
<td>0.00615</td>
<td>0.004103</td>
<td>0.010253</td>
</tr>
<tr>
<td>05/06/83</td>
<td>27</td>
<td>77</td>
<td>3.14</td>
<td>0.00306</td>
<td>0.00360</td>
<td>0.005302</td>
<td>0.008902</td>
</tr>
<tr>
<td>12/06/83</td>
<td>20</td>
<td>34</td>
<td>1.75</td>
<td>0.00804</td>
<td>0.00569</td>
<td>0.010682</td>
<td>0.016372</td>
</tr>
<tr>
<td>24/06/83</td>
<td>26</td>
<td>59</td>
<td>1.56</td>
<td>0.00525</td>
<td>0.00730</td>
<td>0.003153</td>
<td>0.010453</td>
</tr>
<tr>
<td>27/06/83</td>
<td>30</td>
<td>71</td>
<td>1.17</td>
<td>0.00723</td>
<td>0.00695</td>
<td>0.001318</td>
<td>0.008268</td>
</tr>
<tr>
<td>1600 m</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>18/05/83</td>
<td>40</td>
<td>166</td>
<td>4.05</td>
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<td>0.001323</td>
<td>0.002053</td>
</tr>
<tr>
<td>26/05/83</td>
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<td>44</td>
<td>1.80</td>
<td>0.00325</td>
<td>0.00318</td>
<td>0.003886</td>
<td>0.007066</td>
</tr>
<tr>
<td>05/06/83</td>
<td>27</td>
<td>77</td>
<td>3.02</td>
<td>0.00132</td>
<td>0.00135</td>
<td>0.005222</td>
<td>0.006572</td>
</tr>
<tr>
<td>12/06/83</td>
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<td>34</td>
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<td>0.010121</td>
<td>0.013791</td>
</tr>
<tr>
<td>24/06/83</td>
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<td>0.00338</td>
<td>0.00189</td>
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</tr>
<tr>
<td>27/06/83</td>
<td>30</td>
<td>71</td>
<td>1.15</td>
<td>0.00252</td>
<td>0.00284</td>
<td>0.001306</td>
<td>0.004146</td>
</tr>
<tr>
<td>3200 m</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>18/05/83</td>
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<td>166</td>
<td>3.65</td>
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<td>0.00122</td>
<td>0.00183</td>
</tr>
<tr>
<td>26/05/83</td>
<td>26</td>
<td>44</td>
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<td>0.00300</td>
<td>0.003875</td>
<td>0.006875</td>
</tr>
<tr>
<td>05/06/83</td>
<td>27</td>
<td>77</td>
<td>2.84</td>
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<td>0.005129</td>
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<tr>
<td>12/06/83</td>
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<td>34</td>
<td>1.31</td>
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<td>0.008444</td>
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<td>24/06/83</td>
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<td>0.002367</td>
<td>0.005187</td>
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<tr>
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<td>71</td>
<td>1.10</td>
<td>0.00125</td>
<td>0.00121</td>
<td>0.001267</td>
<td>0.002477</td>
</tr>
</tbody>
</table>

TABLE 4

Statistical evaluation of the proposed model and the Hanford experiments

<table>
<thead>
<tr>
<th>The Hanford Experiments</th>
<th>NMSE</th>
<th>FB</th>
<th>COR</th>
<th>FAC2</th>
</tr>
</thead>
<tbody>
<tr>
<td>800m (power)</td>
<td>0.07</td>
<td>0.02</td>
<td>0.77</td>
<td>0.98</td>
</tr>
<tr>
<td>800 m (Logarithmic)</td>
<td>0.44</td>
<td>0.25</td>
<td>0.42</td>
<td>0.78</td>
</tr>
<tr>
<td>800m (sum)</td>
<td>0.44</td>
<td>-0.55</td>
<td>0.73</td>
<td>1.76</td>
</tr>
<tr>
<td>1600m (power)</td>
<td>0.08</td>
<td>0.14</td>
<td>0.86</td>
<td>0.87</td>
</tr>
<tr>
<td>1600 m (Logarithmic)</td>
<td>0.43</td>
<td>0.37</td>
<td>0.51</td>
<td>0.69</td>
</tr>
<tr>
<td>1600m (sum)</td>
<td>0.33</td>
<td>-0.44</td>
<td>0.80</td>
<td>1.56</td>
</tr>
<tr>
<td>3200m (power)</td>
<td>0.08</td>
<td>0.02</td>
<td>0.86</td>
<td>0.98</td>
</tr>
<tr>
<td>3200 m (Logarithmic)</td>
<td>0.20</td>
<td>-0.23</td>
<td>0.86</td>
<td>1.26</td>
</tr>
<tr>
<td>3200m (sum)</td>
<td>0.93</td>
<td>-0.77</td>
<td>0.91</td>
<td>2.24</td>
</tr>
</tbody>
</table>
Fig. 1. Calculated $C_r/Q$ 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 $C_r/Q$ 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 \( C_p/Q \) 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 \( C_p/Q \) 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).

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

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

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

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

where, \( \sigma_p \) and \( \sigma_o \) are the standard deviations of proposed (\( C_p = C_{prod}/Q \)) 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.

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