Maximum crosswind integrated ground level concentration in two stability classes

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1. Introduction

The analytical solution of the atmospheric diffusion equation contains different shapes depending on Gaussian and non-Gaussian solutions. An analytical solution with power law for wind and eddy diffusivity with the realistic assumption was studied by (Demuth, 1978). The solution has been implemented in the KAPPA-G model (Zannetti, 1986; Tirabassi et al., 1986). (Lin and Hildemann, 1997) extended the solution of (Demuth, 1978) under boundary conditions suitable for dry deposition at the ground. The mathematics of atmospheric dispersion modeling is studied by (John, 2011). In the analytical solutions of the diffusion-advection equation, assuming constant along the whole planetary boundary layer (PBL) or following a power law was studied by (Van Ulden and Hotslag, 1978; Pasquill and Smith, 1983; Seinfeld, 1986; Tirabassi et al., 1986; Sharan et al., 1996).

Estimation of crosswind integrated Gaussian and non-Gaussian concentration through different dispersion schemes is studied by (Essa and Fouad, 2011). Analytical solution of diffusion equation in two dimensions using two forms of eddy diffusivities is studied by Essa et al. (2011).

In this paper the advection diffusion equation (ADE) is solved in two directions to obtain crosswind integrated ground level concentration in neutral and unstable conditions. Laplace transformation technique and considering the wind speed and eddy diffusivity depending on the vertical height. Also the ground level and maximum concentrations are estimated. We use in this model empirical data from Copenhagen (Denmark) to compare between predicted and observed concentration data.

2. Analytical solution

Time dependent advection – diffusion equation is written as (Arya, 1995).

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

(1)

where,

- \(x\) is along wind coordinate measured in wind direction from the source (m).
- \(y\) is the crosswind coordinate direction (m).
$z$ is vertical coordinate measured from the ground (m).

$C(x, y, z)$ is the mean concentration of diffusing substance at a point $(x, y, z)$ ($\mu$g/m$^3$).

$k_x$, $k_y$, and $k_z$ are the eddy diffusivity coefficients along $x$, $y$, and $z$ respectively (m$^2$/s).

For steady state, taking $dc/dt = 0$ and neglecting diffusion in the $x$-axis direction because it is small with respect to the advection in the same direction, then Eqn. 1 becomes as follows:

$$u \frac{\partial C}{\partial x} = \frac{\partial}{\partial y} \left( k_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( k_z \frac{\partial C}{\partial z} \right)$$  \hspace{1cm} (2)

Integrating Eqn. (2) with respect to $y$, we obtain the normalized crosswind integrated concentration $C_y(x, z)$ of contaminant at a point $(x, z)$ of the atmospheric advection-diffusion equation in the form (Essa et al., 2006):

$$u(z) \frac{\partial C_y}{\partial x} = k_z \frac{\partial^2 C_y}{\partial^2 z} + \left( \frac{\partial C_y}{\partial z} \right) \left( \frac{\partial k_z}{\partial z} \right)$$ \hspace{1cm} (3)

The above equation is solved in neutral and unstable stabilities using two different schemes for the eddy diffusivity as follows:

A. In neutral case

Taking $k(z) = k_v w^* z$ \hspace{1cm} (4)

where $k_v$ is the von-Karman constant and $w^*$ is the scale vertical velocity.

Substituting from equation (4) in equation (3), we obtain that:

$$\frac{\partial C_y}{\partial x} = k_v w^* z \frac{\partial^2 C_y}{\partial^2 z} + \frac{k_v w^*}{u(z)} \left( \frac{\partial C_y}{\partial z} \right)$$ \hspace{1cm} (5)

Applying the Laplace transform on Eqn. 5 with respect to $x$, we obtain that:

$$\tilde{C}_y(s, z) = L_p \left[ c_y(x, z); x \rightarrow s \right]$$ \hspace{1cm} (6)

where $L_p$ is the operator of the Laplace transform

Substituting from Eqn. 6 in Eqn. 5, we get that:

$$\frac{\partial^2 \tilde{C}_y(s, z)}{\partial z^2} + \frac{1}{z} \frac{\partial \tilde{C}_y(s, z)}{\partial z} - \frac{u}{k_v w^* z} \tilde{C}_y(s, z) = -\frac{u}{k_v w^* z} C_y(0, z)$$ \hspace{1cm} (7)

Equation (3) is subjected to the following boundary condition

(a) The flux at ground and top of the mixing layer can be given by:

$$k_z \frac{\partial C_y}{\partial z} = 0 \text{ at } z = 0, h$$ \hspace{1cm} (i)

(b) The mass continuity is written in the form:

$$u(z) C_y(x, z) = Q \delta(z - h_s) \text{ at } x = 0$$ \hspace{1cm} (ii)

where $\delta$ is Dirac delta function, $Q$ is the source strength and $h_s$ is the stack height.

(c) The concentration of the pollutant tends to zero at large distance of the source, i.e.,

$$C_y(x, z) = 0 \text{ at } x, z \rightarrow \infty$$ \hspace{1cm} (iii)

Substituted from (ii) in equation (7) we obtain that:

$$\frac{\partial^2 \tilde{C}_y(s, z)}{\partial z^2} + \frac{1}{z} \frac{\partial \tilde{C}_y(s, z)}{\partial z} = \frac{-Q}{k_v w^* z} \delta(z - h_s)$$ \hspace{1cm} (8)

Integrated Eqn. (8) with respect to $z$, we obtain that:

$$\frac{\partial \tilde{C}_y(s, z)}{\partial z} = \frac{-Q s \ln(z)}{k_v w^* \delta(z - h_s)}$$ \hspace{1cm} (9)
Equation (9) is a non-homogeneous differential equation. This equation has two solutions: one is homogeneous and the other is the special solution. To solve the homogeneous equation, we put \( -Q / (k_v w_s h_s) = 0 \) in equation 9, then the solution becomes:

\[
\frac{\tilde{C}_y(s, z)}{Q} = c_1 e^{\left(\frac{sw \ln z}{k_v w_s}\right)^z}
\]  

(10)

After taking the Laplace transform in equation (10) and substituting from (ii), we obtain:

\[
c_1 = \frac{1}{us} \delta(z - h_s)
\]  

(11)

Substituting from equation (11) in equation (10) we obtain:

\[
\frac{\tilde{C}_y(s, z)}{Q} = \frac{1}{us} e^{\left(\frac{sw \ln h_s}{k_v w_s}\right)^z}
\]  

(12)

The special solution of equation (9) is in the form as follows:

\[
\left(\frac{\partial}{\partial z} - \frac{us \ln(z)}{k_v w_s}\right) \tilde{C}_y(s, z) = -\frac{Q}{k_v w_s h_s}
\]

\[
\Rightarrow \frac{\tilde{C}_y(s, z)}{Q} = \frac{1}{k_v w_s h_s} \left( D - \frac{us \ln(z)}{k_v w_s} \right)
\]  

(13)

where, \( D = \frac{\partial}{\partial z} \)

Then solution of equation (13) is in the form as follows:

\[
\frac{\tilde{C}_y(s, z)}{Q} = \frac{1}{us h_s \ln h} e^{\left(-\frac{u(h \ln h - z \ln z)}{k_v w_s}\right)}
\]  

(14)

The general solution of equation (13) is given by summing two solutions equations (14) and (12) in the form:

\[
\frac{\tilde{C}_y(s, z)}{Q} = \frac{1}{us} e^{\left(\frac{sw \ln h_s}{k_v w_s}\right)^z} + \frac{1}{us h_s \ln h} e^{\left(-\frac{u(h \ln h - z \ln z)}{k_v w_s}\right)}
\]  

(15)

Taking Laplace inverse on Eqn. (15), we get:

\[
\frac{C_y(x, z)}{Q} = \frac{1}{u} \left[ x - \frac{uh_s \ln(h_s)}{k_v w_s} \right] + \frac{1}{u h_s \ln(h)} \left\{ x - \frac{uh \ln(h) - z \ln(z)}{k_v w_s} \right\}
\]  

(16)

Since:

\[
L^{-1}(AB) = L^{-1}(A)L^{-1}(B) \quad L^{-1}\left(\frac{1}{s}\right) = 1,
\]

\[
L^{-1}\left[\exp(-as)\right] = \frac{1}{x + a} \quad \text{and} \quad L^{-1}\left[\exp(as)\right] = \frac{1}{x - a}
\]

\( L^{-1} \) is the operator of the inverse Laplace transform by (Shamus, 1980). To calculate the integrated ground level concentration, we put \( z = 0 \) in Eqn. (16), we get:

\[
\frac{C_y(x, 0)}{Q} = \frac{1}{u} \left[ x - \frac{uh_s \ln(h_s)}{k_v w_s} \right] + \frac{1}{u h_s \ln(h)} \left\{ x - \frac{uh \ln(h) - z \ln(z)}{k_v w_s} \right\}
\]  

(17)
Differentiating Eqn. (17) with respect to \(x\) and equating the result to zero, we get the maximum downwind distance in the form:

\[
x_{max} = \frac{u \left[ \sqrt{h_s \ln(h)} (h - h_y) \ln(h) \right]}{k_v w_* [1 + \sqrt{h_s \ln(h)}]}
\]  

(18)

Substituting from Eqn. (18) in Eqn. (17), we get the maximum crosswind integrated ground level concentration as follows:

\[
\frac{C_{max} (x, 0)}{Q} = \frac{1}{u} \left\{ \frac{u (h_x - h) \ln(h) [h_s \ln(h)]^{1/2}}{k_v w_* [1 + \sqrt{h_s \ln(h)}]} - \frac{u h_x \ln(h)}{k_v w_*} \right\}
\]  

(19)

B. In unstable case

In unstable case we take the value of the vertical eddy diffusivity in the form:

\[
k(z) = k_v w_* z \ (1-z/h)
\]  

(20)

Substituting from equation (20) in equation (3), we get that:

\[
\frac{\partial C_y}{\partial x} = k_v w_* z \left( \frac{1-z}{h} \right) \frac{\partial^2 C_y}{\partial z^2} + k_v w_* \left( \frac{1-2z}{h} \right) \frac{\partial C_y}{\partial z}
\]  

(21)

After integrating equation (24) with respect to \(z\), we obtain that:

\[
L_p \left( \frac{\partial C_y}{\partial x} \right) = sC_y (s, z) - C_y (0, z)
\]  

(22)

where \(L_p\) is the operator of the Laplace transform

Substituting from Eqn. (22) in Eqn. (21), we obtain that:

\[
\frac{\partial^2 C_y}{\partial z^2} + \left( \frac{1-2z}{h} \right) \frac{\partial^2 C_y}{\partial z} - \frac{us}{k_v w_* \left( \frac{z-z^2}{h} \right)} C_y (s, z) = 0
\]  

(23)

Substituting from (ii) in Eqn. 23 we get:

\[
\frac{\partial^2 C_y (s, z)}{\partial z^2} + \left( \frac{1-2z}{h} \right) \frac{\partial^2 C_y (s, z)}{\partial z} - \frac{us}{k_v w_* \left( \frac{z-z^2}{h} \right)} C_y (s, z) = \frac{Q^i(z-h)}{k_v w_* \left( \frac{z-z^2}{h} \right)}
\]  

(24)

Eqn. (25) is non-homogeneous differential equation then, above equation has got two solutions, one is homogeneous and other is special solution, in order to solve the homogeneous, we put, \(-Q = 0\) in

\[
\frac{Q}{k_v w_* \left( 1-h/\h_s \right)} = 0
\]  

(25)

Eqn. (25), the solution becomes:
\[ \frac{\tilde{C}_y(s, z)}{Q} = c_se^{-\left(\frac{su \ln\frac{z-h}{z}}{k_\nu w_s}\right)z} \]  

(26)

After taking Laplace transform in equation (26) and substitute from (ii), we obtain that:

\[ c_z = \frac{1}{us} \delta(z-h_t) \]  

(27)

Substituting from equation (27) in equation (26) we get that:

\[ \frac{\tilde{C}_y(s, z)}{Q} = \frac{1}{us} e^{-\left(\frac{su \ln\frac{h_t-h}{h_t}}{k_\nu w_s}\right)z} \]  

(28)

The special solution of equation (25) becomes:

\[ \frac{\tilde{C}_y(s, z)}{Q} = \frac{1}{k_\nu w_s h_t \left(\frac{h_t}{h} - 1\right)} e^{-\left(\frac{su \ln\frac{z-h}{z}}{k_\nu w_s}\right)z} \]  

(29)

Then, the general solution of eqn. (25) is as follows:

\[ \frac{\tilde{C}_y(s, z)}{Q} = \frac{1}{us} e^{-\left(\frac{su \ln\frac{z-h}{z}}{k_\nu w_s}\right)z} \]  

(30)

Taking Laplace inverse of equation (30), we get that:

\[ \frac{C_y(x, z)}{Q} = \frac{1}{u \ln\frac{h_t-h}{h_t}} \left\{ \frac{u \ln\frac{z-h}{z}}{x - \frac{u \ln\frac{z-h}{z}}{k_\nu w_s}} + \frac{1}{k_\nu w_s h_t \left(\frac{h_t}{h} - 1\right) \left(\frac{u \ln\frac{z-h}{z}}{x - \frac{u \ln\frac{z-h}{z}}{k_\nu w_s}} - \frac{1}{x-a}\right)} \right\} \]  

(31)

Since:

\[ L^{-1}(AB) = L^{-1}(A)L^{-1}(B) \quad L^{-1}\left(\frac{1}{s}\right) = 1, \]  

\[ L^{-1}\left[\exp\left(-as\right)\right] = \frac{1}{x+a} \quad \text{and} \quad L^{-1}\left[\exp\left(\frac{as}{s}\right)\right] = \frac{1}{x-a} \]

L^{-1} is the operator of the Laplace inverse transform by (Shamus, 1980).

To get the crosswind integrated ground level concentration, we put \( z = 0 \) in Eqn. 31, we get that:

\[ \frac{C_y(x,0)}{Q} = \frac{1}{u \ln\frac{h_t-h}{h_t}} \left\{ \frac{u \ln\frac{h_t-h}{h_t}}{x - \frac{u \ln\frac{h_t-h}{h_t}}{k_\nu w_s}} + \frac{1}{k_\nu w_s h_t \left(\frac{h_t}{h} - 1\right) \left(\frac{u \ln\frac{h_t-h}{h_t}}{x - \frac{u \ln\frac{h_t-h}{h_t}}{k_\nu w_s}} - \frac{1}{x-a}\right)} \right\} \]  

(32)

Differentiating Eqn. (32) with respect to \( x \) and equating it to zero, we get on the maximum downwind distance as follows:

\[ x_{\text{max}} = \frac{u \ln\frac{h_t-h}{h_t}}{k_\nu w_s \left\{ \left(\frac{h_t}{h} - 1\right) - \sqrt{u} \right\}} \]  

(33)
TABLE 1
Comparison between observed, predicted and maximum normalized crosswind integrated ground level concentrations under different stabilities, mixing height, wind speed and maximum downwind distance

<table>
<thead>
<tr>
<th>Run no.</th>
<th>Stability</th>
<th>h(m)</th>
<th>U (m/s)</th>
<th>distance (x) (m)</th>
<th>w*</th>
<th>C_{x,h} (x, 0) \times 10^4 (s/m^2)</th>
<th>x_{max}</th>
<th>x/h</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Very unstable (A)</td>
<td>1980</td>
<td>3.34</td>
<td>1900</td>
<td>1.8</td>
<td>6.48</td>
<td>5.01</td>
<td>2.15</td>
</tr>
<tr>
<td>1</td>
<td>Very unstable (A)</td>
<td>1980</td>
<td>3.34</td>
<td>3700</td>
<td>1.8</td>
<td>2.31</td>
<td>2.62</td>
<td>1.30</td>
</tr>
<tr>
<td>2</td>
<td>Slightly unstable (C)</td>
<td>1920</td>
<td>7.79</td>
<td>2100</td>
<td>1.8</td>
<td>5.38</td>
<td>4.36</td>
<td>2.51</td>
</tr>
<tr>
<td>2</td>
<td>Slightly unstable (C)</td>
<td>1920</td>
<td>7.79</td>
<td>4200</td>
<td>1.8</td>
<td>2.95</td>
<td>2.26</td>
<td>1.41</td>
</tr>
<tr>
<td>3</td>
<td>Moderately unstable (B)</td>
<td>1120</td>
<td>3.82</td>
<td>1900</td>
<td>1.3</td>
<td>8.2</td>
<td>5.01</td>
<td>5.89</td>
</tr>
<tr>
<td>3</td>
<td>Moderately unstable (B)</td>
<td>1120</td>
<td>3.82</td>
<td>3700</td>
<td>1.3</td>
<td>6.22</td>
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<td>1120</td>
<td>3.82</td>
<td>5400</td>
<td>1.3</td>
<td>4.3</td>
<td>1.80</td>
<td>2.30</td>
</tr>
<tr>
<td>5</td>
<td>Slightly unstable (C)</td>
<td>820</td>
<td>4.93</td>
<td>2100</td>
<td>0.7</td>
<td>6.72</td>
<td>4.50</td>
<td>10.74</td>
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<tr>
<td>5</td>
<td>Slightly unstable (C)</td>
<td>820</td>
<td>4.93</td>
<td>4200</td>
<td>0.7</td>
<td>5.84</td>
<td>2.27</td>
<td>7.12</td>
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<tr>
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<td>4.93</td>
<td>6100</td>
<td>0.7</td>
<td>4.97</td>
<td>1.57</td>
<td>4.42</td>
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<td>11.45</td>
<td>2000</td>
<td>2</td>
<td>3.96</td>
<td>4.35</td>
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<td>Slightly unstable (C)</td>
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<td>11.45</td>
<td>4200</td>
<td>2</td>
<td>2.22</td>
<td>2.21</td>
<td>1.42</td>
</tr>
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<td>Slightly unstable (C)</td>
<td>1300</td>
<td>11.45</td>
<td>5900</td>
<td>2</td>
<td>1.83</td>
<td>1.60</td>
<td>0.85</td>
</tr>
<tr>
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<td>Moderately unstable (B)</td>
<td>1850</td>
<td>6.52</td>
<td>2000</td>
<td>2.2</td>
<td>6.7</td>
<td>4.57</td>
<td>1.58</td>
</tr>
<tr>
<td>7</td>
<td>Moderately unstable (B)</td>
<td>1850</td>
<td>6.52</td>
<td>4100</td>
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<td>2.32</td>
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<tr>
<td>7</td>
<td>Moderately unstable (B)</td>
<td>1850</td>
<td>6.52</td>
<td>5300</td>
<td>2.2</td>
<td>2.23</td>
<td>1.81</td>
<td>0.62</td>
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<td>8</td>
<td>Neutral (D)</td>
<td>810</td>
<td>6.68</td>
<td>1900</td>
<td>2.2</td>
<td>4.16</td>
<td>4.89</td>
<td>0.02</td>
</tr>
<tr>
<td>8</td>
<td>Neutral (D)</td>
<td>810</td>
<td>6.68</td>
<td>3600</td>
<td>2.2</td>
<td>2.02</td>
<td>2.68</td>
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<tr>
<td>8</td>
<td>Neutral (D)</td>
<td>810</td>
<td>6.68</td>
<td>5300</td>
<td>2.2</td>
<td>1.52</td>
<td>1.85</td>
<td>0.07</td>
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<tr>
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<td>Slightly unstable (C)</td>
<td>2090</td>
<td>8.11</td>
<td>2100</td>
<td>1.9</td>
<td>4.58</td>
<td>4.34</td>
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</tr>
<tr>
<td>9</td>
<td>Slightly unstable (C)</td>
<td>2090</td>
<td>8.11</td>
<td>4200</td>
<td>1.9</td>
<td>3.11</td>
<td>2.26</td>
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</tr>
<tr>
<td>9</td>
<td>Slightly unstable (C)</td>
<td>2090</td>
<td>8.11</td>
<td>6000</td>
<td>1.9</td>
<td>2.59</td>
<td>1.60</td>
<td>0.70</td>
</tr>
</tbody>
</table>

Substituting from Eqn. (33) in Eqn. (32), we get the maximum crosswind integrated ground level concentration as follows:

\[
C_{x,h}(x, 0) = \frac{1}{Q} \left( \frac{u h}{k_w h} \right) \left( \frac{u h}{k_w h} \right) \left( 1 - \frac{h}{h} \right) \left( -\sqrt{\frac{u}{w}} \right) \left( \frac{u h}{k_w h} \right) \left( \frac{u h}{k_w h} \right) \left( 1 - \frac{h}{h} \right) \left( -\sqrt{\frac{u}{w}} \right)
\]

The data used was observed from the atmospheric diffusion experiments conducted at the northern part of Copenhagen, Denmark, under neutral and unstable conditions (Gryning and Lyck, 1984; Gryning et al., 1987). Table 1 shows the comparison between observed, predicted and maximum integrated crosswind ground level concentrations under different stabilities, mixing height, wind speed and maximum downwind distance.

Fig. 1. Shows comparison between the observed, predicted and maximum normalized crosswind integrated ground level concentrations under different stabilities.

Fig. 2. Shows comparison between the observed, predicted and maximum normalized crosswind integrated...
3. Statistical method

Now, the statistical method is presented and comparison between predicted and observed results will be offered by (Hanna, 1989). The following standard statistical performance measures that characterize the agreement between prediction \( (C_p = C_{pred}/Q) \) and observations \( (C_o = C_{obs}/Q) \):

\[
\text{Fractional Bias (FB)} = \frac{\bar{C_o} - \bar{C_p}}{0.5(\bar{C_o} - \bar{C_p})}
\]

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

\[
\text{Correlation Coefficient (COR)} = \frac{\sum_{i=1}^{N} (C_{pi} - \bar{C_p}) \times (C_{oi} - \bar{C_o})}{\sigma_p \sigma_o}
\]

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

Where \( \sigma_p \) and \( \sigma_o \) are the standard deviations of \( C_p \) and \( C_o \) respectively. Here the over bars indicate the average over all measurements. A perfect model would have the following idealized performance: \( \text{NMSE} = \text{FB} = 0 \) and \( \text{COR} = 1.0 \).

From the statistical method, we find that the two models are within a factor of two with observed data. According to NMSE and FB, the predicted normalized crosswind integrated ground level concentration is better than maximum normalized crosswind integrated ground level concentration. The correlation of predicated model equals (0.67) and maximum model equals (0.70) (Table 2).

4. Conclusions

This method solving Laplace transforms technique and eddy diffusivity depends on the vertical height in ground level concentrations under different stability via downwind distance over height.
neutral and unstable conditions. Also the predicted and maximum normalized crosswind integrated ground level concentrations are estimated. We find that the predicted and maximum normalized crosswind integrated concentrations are within a factor of two with observed concentration data. One finds that there is agreement between maximum and predicted normalized crosswind integrated concentrations with the observed normalized crosswind integrated concentrations.

**TABLE 2**

<table>
<thead>
<tr>
<th>Models</th>
<th>NMSE</th>
<th>FB</th>
<th>COR</th>
<th>FAC2</th>
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</thead>
<tbody>
<tr>
<td>Predicted concentration</td>
<td>0.26</td>
<td>0.32</td>
<td>0.67</td>
<td>0.80</td>
</tr>
<tr>
<td>Maximum concentration</td>
<td>0.62</td>
<td>0.52</td>
<td>0.70</td>
<td>0.51</td>
</tr>
</tbody>
</table>

References


Shamus, 1980, “Theories and examples in Mathematics for Engineering and Scientific”.


