ANALYTICAL SOLUTION OF DIFFUSION EQUATION IN TWO DIMENSIONS USING TWO FORMS OF EDDY DIFFUSIVITIES

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An analytical solution of the two-dimensional atmospheric diffusion equation has been developed by the method of Separation of variables. Also Fourier transform and square complement methods has been used to solve the integration. The present model is validated with the data sets obtained at the Northern part of Copenhagen (Gryning and Lyck, 1984) of the tracer sulfur hexafluoride (SF₆) in unstable conditions. In this model the vertical eddy diffusivity depends on the downwind distance and is calculated using two methods \( \kappa(x) = \gamma Ux \), and \( \kappa(x) = \kappa_0 Ux \). Values of the calculated normalized crosswind concentration are calculated differently, according to the different eddy diffusivities. These values are compared with the observed data graphically and statistically. The proposed method No.1 has performed better than method No.2 with the data from the diffusion experiment considered.

1. INTRODUCTION

Efforts are exerted to the task of searching analytical solutions for the advection-diffusion equation in order to simulate the pollutant dispersion in the atmospheric boundary layer (ABL). A dispersion model of pollutants released from continuous source is presented. The model is based on the bi-dimensional semi-empirical equation and the novelty consists on the derivation and application of profiles of wind speed and eddy diffusivity.

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 ABL or follow a power law (van Ulden, 1978; Pasqual and Smith, 1983; Seinfeld, 1986; Tirabassi et al., 1986; Sharan et al., 1996). Moriera et al., (2005) presented a solution of the advection-diffusion equation based on the Laplace transform considering the ABL as a multilayer system.
Number of dispersion regulatory models include improved dispersion algorithms in terms of fundamental scaling parameters (Cosemans et al., 1992; Olesen et al., 1992; Hanna and Chang, 1993; Carruthers et al., 1995). Gryning et al. (1987) suggested a modeling approach composed by individual models, each one based the specific turbulent structure of the regimes in the ABL, following Holtslag and Nieuwstadt (1986). 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. (1982) 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. 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.

In this work, an analytical solution of the two-dimensional atmospheric diffusion equation has been developed by the method of Separation of variables. Also Fourier transform and square complement methods has been used to solve the integration. The present model is validated with the data sets obtained at the Northern part of Copenhagen (Gryning and Lyck, 1984) of the tracer sulfur hexafluoride (SF$_6$) in unstable conditions. In this model the vertical eddy diffusivity depends on the downwind distance and is calculated using two methods $K(x) = \gamma U x$, and $K(x) = K_0 U x$. Values of the calculated normalized crosswind concentration are calculated differently, according to the different eddy diffusivities. These values are compared with the observed data graphically and statistically.

2. MATHEMATICAL MODEL

The Diffusion equation in three dimensions is

$$ U \frac{\partial C}{\partial x} = \frac{\partial}{\partial z} \left( K(z) \frac{\partial C}{\partial z} \right) + \frac{\partial}{\partial y} \left( K(y) \frac{\partial C}{\partial y} \right) $$

(1)

where,
- $C$ is the concentration of pollutants (µg/m$^3$)
- $U$ is the wind speed (m/s)
- $K(z)$ and $K(y)$ are the eddy diffusivities in vertical and crosswind directions respectively.
- $x$, $y$, and $z$ are the Cartesian coordinates in downwind, crosswind, and vertical directions.
By taking crosswind integration with respect to y from \(-\infty\) to \(\infty\), we get diffusion equation in two dimensions as follows:

\[
U \frac{\partial C_y}{\partial x} = -\frac{\partial}{\partial x} \left( K(x) \frac{\partial C_y}{\partial x} \right)
\]

(2)

where,

\(K(x)\) is the eddy diffusivity which is a function depends on the downwind distance.

Using the boundary conditions to solve the diffusion equation in two dimensions;

1 – The mass is conservative

\[UC_y(x, z, h) = Q \delta(x - h), \forall x = 0\]

(3)

where, \(h\) is the mixing height, \(\delta(z-h)\) is the Dirac delta function.

The concentration tends to zero when \(x\) and \(z\) tend to infinity.

\[C = 0 \quad \text{at} \quad x \text{ and } z \rightarrow \infty\]

(4)

Eqn (2) is solved by using the Separation of variables method,

\[C_y(x, z, h) = S(x)R(z, h)\]

(5)

By substituting from Eqn (5) in Eqn (2), we get

\[
UR(z, h) \frac{dS}{dx} = K(x)S(x) \frac{d^2R}{dx^2}
\]

(6)

Divide both sides over \(S(x)\) \(R(z,h)\)

\[
\frac{U}{S(x)} \frac{dS}{dx} = \frac{K(x)}{R(z, h)} \frac{d^2R}{dx^2}
\]

(7)

Let’s equal both sides to \(-P^2\):

\[
\frac{1}{S(x)} \frac{dS}{dx} = \frac{K(x)}{UR(z, h)} \frac{d^2R}{dx^2} = -P^2
\]

(8)

then,

\[
\frac{1}{S(x)} \frac{dS}{dx} = -P^2
\]

\[
\int \frac{dS}{S(x)} = \int -P^2 \, dx
\]
\[
\ln S(x) = -P^2 x + \ln g
\]
where \( g \) is a constant.

\[
\ln \frac{S(x)}{g} = -P^2 x
\]
\[
\frac{S(x)}{g} = e^{-P^2 x}
\]

So,
\[
S(x) = g e^{-P^2 x}
\]

(9)

Also,
\[
\frac{K(x)}{UR(z, h)} \frac{\partial^2 H}{\partial x^2} = -P^2
\]
\[
\frac{\partial^2 R}{\partial z^2} = \frac{U P^2}{K} R(x, h)
\]

and,
\[
R(z, h) = A(h) e^{\frac{P z}{\sqrt{K}}} + B(h) e^{-\frac{P z}{\sqrt{K}}}
\]
(10)

Where \( A(h) \) and \( B(h) \) are constants depend on the mixing height.

Then we can write Eqn (4) in the form:

\[
C_y(x, z, h) = g A(h) e^{-\frac{P x + \frac{P z}{\sqrt{K}}}{\sqrt{K}}} + g B(h) e^{-\frac{P x - \frac{P z}{\sqrt{K}}}{\sqrt{K}}}
\]
(11)

Each term in this equation is oscillatory but bounded as \( z \to \pm \infty \) for all distances \( x \geq 0 \).

\[
\lim_{z \to \pm \infty} \frac{L H n}{x} C_y A(h) e^{-\frac{P x + \frac{P z}{\sqrt{K}}}{\sqrt{K}}} = \text{Oscillatory}
\]
(12)

\[
\lim_{z \to \pm \infty} \left| g A(h) e^{-\frac{P x + \frac{P z}{\sqrt{K}}}{\sqrt{K}}} \right| = g A(h) e^{-P x}
\]

Also,

\[
\lim_{z \to \pm \infty} \left| g B(h) e^{-\frac{P x - \frac{P z}{\sqrt{K}}}{\sqrt{K}}} \right| = g B(h) e^{-P x}
\]
(13)
Since \( 0 < P < \infty \) varies continuously, the sum of all these solutions depends on the integration of \( P \). So, the general solution is:

\[
C_y(x, z, h) = \int_0^\infty g(P)A(P, h)e^{-\frac{R^2}{P} + \frac{PR}{P}} dP + \int_0^\infty g(P)B(P, h)e^{-\frac{R^2}{P} - \frac{PR}{P}} dP
\]

Also we can write Eq. (14) in the form:

\[
C_y(x, z, h) = \int_{-\infty}^\infty \left[ g(P)A(P, h) + g(-P)B(-P, h) \right] e^{\frac{R^2}{P} + \frac{PR}{P}} dP
\]

Let,

\[
V(P, h) = g(P)A(P, h) + g(-P)B(-P, h)
\]

\[
V(P, h) = g(P)g(P, h)
\]  

if \( P > 0 \)

\[
V(P, h) = g(-P)B(-P, h)
\]  

if \( P < 0 \)

Eqn (16) becomes:

\[
C_y(x, z, h) = \int_{-\infty}^\infty V(P, h) e^{-\frac{R^2}{P} + \frac{PR}{P}} dP
\]

To find the value of \( V(P, h) \), use the Fourier Transform of \( \delta(z-h) \) as follows:

Fourier transform \( \delta(z-h) \) is:

\[
g(P) = \int_{-\infty}^{\infty} \delta(z-h)e^{-iPz} dz
\]

\[
g'(P) = e^{-iP\sqrt{K}}
\]

Let,

\[
P \sqrt{\frac{K}{\rho}} = w \quad \text{and} \quad dP = \sqrt{\frac{K}{\rho}} dw
\]

\[
g(P) = e^{-iwK}
\]
By using Square compliment method to solve the integration:

\[
\delta(x - h) = \int_{-\infty}^{\infty} e^{-iw(x-h)} \sqrt{\frac{K}{U}} \frac{dw}{2\pi}
\]

(22)

By substituting \(\delta(z-h)\) with its value in Eqn (23), we find that:

\[
\int_{-\infty}^{\infty} e^{-iw(z-h)} \frac{dw}{2\pi} \sqrt{\frac{K}{U}} = \int_{-\infty}^{\infty} V(P, h) e^{-iwz} dw \sqrt{\frac{K}{U}}
\]

(24)

By substituting \(\delta(z-H)\) with its value in Eqn (23), we find that;

\[
\int_{-\infty}^{\infty} e^{-iw(z-h)} \frac{dw}{2\pi} \sqrt{\frac{K}{U}} = \int_{-\infty}^{\infty} V(P, h) e^{-iwz} dw \sqrt{\frac{K}{U}}
\]

(25)

So,

\[
V(P, h) = \frac{Q}{2\pi U} e^{-iwh}
\]

(26)

Then Eqn (17) can be written in the form:

\[
L_j(x, u, h) = \frac{Q}{U} \int_{-\infty}^{\infty} e^{-P^2 x + iP(x-h), \frac{P}{2}, \frac{4P}{2\pi}}
\]

(27)

By using Square compliment method to solve the integration:

\[
P^2 x - iP \sqrt{\frac{U}{K}}(x-h) = \left\{ P^2 - \frac{iP}{\sqrt{\frac{K}{U}}} (x-h) \right\}^{\frac{1}{2}}
\]

(28)

\[
P^2 x - iP \sqrt{\frac{U}{K}}(x-h) = \left\{ P^2 - \frac{iP}{2\sqrt{\frac{K}{U}}} (x-h) \right\}^{\frac{1}{2}} - \left\{ \frac{i}{2\sqrt{\frac{K}{U}}} (x-h) \right\}^{\frac{1}{2}}
\]

(29)
By substituting this formula into the integral in Eqn (27), we find that:

\[ F^2 x - \frac{d}{\sqrt{h}}(x - h) \int \left[ \frac{1}{2x} \left( \frac{y}{\sqrt{h}} \right) \right]^2 \left[ \frac{1}{2x} \left( \frac{y}{\sqrt{h}} \right) \right]^2 \, dP \]

By substituting this formula into the integral in Eqn (27), we find that:

\[ C_y(x, z, h) = \frac{Q}{U} \int e^{-\left( \frac{(y-h)^2}{2\lambda^2} \right)} \int e^{-\left( \frac{(y-h)^2}{2\lambda^2} \right)} \, dP \]

Let,

\[ \sqrt{x} \left( P - \frac{i(x - h) \sqrt{v}}{2x} \right) = n \]

\[ dP = \frac{1}{\sqrt{x}} \, dn \]

\[ C_y(x, z, h) = \frac{Q}{U} e^{-\left( \frac{(y-h)^2}{2\lambda^2} \right)} \int e^{-\left( \frac{(y-h)^2}{2\lambda^2} \right)} \, dn \]

\[ C_y(x, z, h) = \frac{Q}{2U\sqrt{x}} e^{-\left( \frac{(y-h)^2}{2\lambda^2} \right)} \int e^{-\left( \frac{(y-h)^2}{2\lambda^2} \right)} \, dn \]

3. VALIDATION

The present model is validated with the data sets obtained at the Northern part of Copenhagen (Gryning and Lyck, 1984) and from the field experiment conducted at Kincaid (Hudischewskyi and Reynolds, 1983) in unstable conditions.
The tracer sulfur hexafluoride (SF₆) was released from a tower at a height of 115 m without buoyancy. The roughness length was 0.6 m. The values of parameters such as inversion height (h), wind speed at 10 m (U₁₀), \( \sigma_w \) and observed concentration during the experiment (Table 1) are taken from Gryning et al. (1987). The stability is classified on the basis of the values of Monin-Obukhov length L (Sharan and Gupta, 2002). The site was primarily residential, therefore the terrain was considered as an urban terrain for calculation.

In the present model we have used two methods for the calculation of the eddy diffusivity in the downwind distance (k). The first method is referenced to (Area, 1999) where \( K \) takes the form of,

\[
K(x) = \gamma U x = 0.16 \frac{\sigma_w^2}{U} x
\]

where,

\( \gamma \) is a parameter depends on the stability condition and equals to \( \gamma = 0.16 \left( \frac{\sigma_w}{U} \right)^2 \)

<table>
<thead>
<tr>
<th>Run no.</th>
<th>Stability</th>
<th>U₁₀(m.sec⁻¹)</th>
<th>h(m)</th>
<th>Distance (x) (m)</th>
<th>( \sigma_w ) (ms⁻¹)</th>
<th>Observed</th>
<th>Predicted (Model 1)</th>
<th>Predicted (Model 2)</th>
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<td>1</td>
<td>Very unstable (A)</td>
<td>2.1</td>
<td>1980</td>
<td>1900</td>
<td>0.83</td>
<td>6.48</td>
<td>0.075</td>
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<tr>
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<td>0.83</td>
<td>2.31</td>
<td>4.513</td>
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<td>1920</td>
<td>2100</td>
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<td>5.38</td>
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<td>1920</td>
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<td>1.07</td>
<td>2.95</td>
<td>2.801</td>
<td>2.09E-02</td>
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<tr>
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<td>3</td>
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<td>3700</td>
<td>0.68</td>
<td>6.22</td>
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<td>Moderately unstable (B)</td>
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<td>0.68</td>
<td>4.3</td>
<td>12.882</td>
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<td>4000</td>
<td>0.47</td>
<td>11.7</td>
<td>17.322</td>
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<td>3.1</td>
<td>820</td>
<td>2100</td>
<td>0.71</td>
<td>6.72</td>
<td>9.818</td>
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<td>2000</td>
<td>1.33</td>
<td>3.96</td>
<td>0.976</td>
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Table 1 (continued)

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<th>No.</th>
<th>Stability Class</th>
<th>u</th>
<th>w</th>
<th>1/3</th>
<th>1/2</th>
<th>(\sigma_w)</th>
<th>(K)</th>
</tr>
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<td>Slightly unstable (C)</td>
<td>7.2</td>
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<td>1.33</td>
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<td>7.2</td>
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<td>1.83</td>
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<td>2000</td>
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<td>7</td>
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<td>1850</td>
<td>4100</td>
<td>0.87</td>
<td>3.25</td>
<td>3.509</td>
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<tr>
<td>7</td>
<td>Moderately unstable (B)</td>
<td>4.1</td>
<td>1850</td>
<td>5300</td>
<td>0.87</td>
<td>2.23</td>
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<td>8</td>
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<td>810</td>
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<tr>
<td>8</td>
<td>Neutral (D)</td>
<td>4.2</td>
<td>810</td>
<td>3600</td>
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<td>8</td>
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<td>4.2</td>
<td>810</td>
<td>5300</td>
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<td>Slightly unstable (C)</td>
<td>5.1</td>
<td>2090</td>
<td>2100</td>
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<td>2090</td>
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<td>2090</td>
<td>6000</td>
<td>0.98</td>
<td>2.59</td>
<td>3.628</td>
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</tbody>
</table>

\(\sigma_w\) is the scale vertical velocity.

While the second method is referenced to (Hanna et al. 1982) and \(K\) takes the form of,

\[K(x) = k_0 \nu_x \frac{\nu_x}{x} = 0.04(Ux)\]

where,
\(k_0\) is von-Karman constant equals to 0.4
\(\nu_x\) is the fractional velocity and equals to \(\nu_x = 0.1(U)\)

The concentrations Predicted from the present model (Eqn (37)) are also reported in Table 1.

4. COMPARISON BETWEEN THE USED METHODS

In this section, we compared between the final results obtained using the two methods. We look for which is the most optimum method to be used. Fig. 1 shows the relation between the observed and predicted crosswind concentrations of the tracer sulfur hexafluoride (SF6) with downwind distances from continuous source.

From Fig. 1, we find that both models can be considered agree with the observed data except some points.

In the next figure, we plot the normalized predicted crosswind concentrations versus the observed concentrations.
Fig. 1 – The Relation between the downwind distances and the observed and predicted concentrations of SF6.

Fig. 2 – Plot between observed and predicted concentrations for the present model.

Regarding Fig. 2, we can observe that method No.1 has some points near the observed data, while others are over-predicted. In the other hand method No.2 has also some points near the observed data and the others are almost near zero line. This also can appear in Fig. 3.
4.1. STATISTICAL METHOD

Here we seek for knowing which method’s results are the nearest to the observed concentrations. So to solve this problem, we have used the following standard statistical performance measures that characterize the agreement between model prediction \((C_p = C_{pred}/Q)\) and observations \((C_o = C_{obs}/Q)\):

\[
\text{Normalized Mean Square Error (NMSE)} = \frac{(C_o - C_p)^2}{\bar{C_o} \cdot \bar{C_p}} \tag{4.1}
\]

\[
\text{Fractional Bias (FB)} = \frac{\bar{C_o} - \bar{C_p}}{\bar{C_o} + \bar{C_p}} \tag{4.2}
\]

\[
\text{Correlation Coefficient (COR)} = \frac{1}{N_m} \sum_{i=1}^{N_m} (C_{pi} - \bar{C_p}) \times \frac{(C_{oi} - \bar{C_o})}{\sigma_p \cdot \sigma_o} \tag{4.3}
\]

\[
\text{Factor of Two (FAC2)} = 0.5 \leq \frac{C_o}{C_p} \leq 2.0 \tag{4.4}
\]

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 \((N_m)\). A perfect model would have the following idealized performance:

\[
\text{NMSE} = \text{FB} = 0 \text{ and } \text{COR} = \text{FAC2} = 1.0
\]
Table 2

Comparison between the two methods according to standard statistical performance measure

<table>
<thead>
<tr>
<th>Models</th>
<th>NMSE</th>
<th>FB</th>
<th>FAC2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Method No.1</td>
<td>0.95</td>
<td>-0.24</td>
<td>1.59</td>
</tr>
<tr>
<td>Method No.2</td>
<td>1.57</td>
<td>0.69</td>
<td>0.49</td>
</tr>
</tbody>
</table>

From the statistical method, we find that the two methods are factors of 2 with observed data. Regarding to NMSE, the method No.1 is better than the other model. Method No.1 is also the best relating to FB. But the correlation of method No.2 equals (0.51) which is stronger to the observed data than the correlation of method No.1 which equals (0.06).

5. CONCLUSION

We have developed an analytical solution of two-dimensional atmospheric diffusion equation by the method of Separation of variables to calculate normalized crosswind concentrations for continuous source emits (SF₆). In this model the vertical eddy diffusivity depends on the downwind distance and is calculated using two methods

\[ \kappa(x) = v \lambda x, \quad \kappa(x) = \kappa_0 U x. \]

Graphically, we can observe that method No.1 has some points near the observed data, while others are over-predicted. In the other hand method No.2 has also some points near the observed data and the others are almost near zero line.

From the statistical method, we find that the two methods are factors of 2 (FAC2) with observed data. Regarding to NMSE, the method No.1 is better than the other model. Also method No.1 is the best relating to FB.

REFERENCES


