Full length article

Studying the variation of eddy diffusivity on the behavior of advection-diffusion equation

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\textbf{A B S T R A C T}

In this work, the advection-diffusion equation was solved in two dimensions to calculate the normalized crosswind integrated concentration by Laplace technique. Considering that the wind speed is constant and we have two models of the vertical eddy diffusivity, one depends on downwind distance and the other model depends on vertical distance. A comparison between our proposed two models, Gaussian, previous work and observed data measured at Copenhagen, Denmark, have been carried out. One finds that there is a good agreement between predicted (2) model and the observed concentrations than predicted (1), Gaussian and previous work.

From the statistical technique, one finds that all models are inside a factor of two with observed data. Regarding to Normalized mean square error (NMSE) and Fraction Bais (FB), proposed model (2) is performance well with observed data than the predicted (1), Gaussian and previous work in unstable condition.

1. Introduction

It is very important to be aware of how contaminants are dispersed through the atmosphere. Unfortunately, Air pollutants influence directly or indirectly on man and environment. Essa and El-Otaify (2008), Alharbi (2011) discussed the dispersion of pollutant mainly depends on meteorological and topographical conditions. In order to understand the dispersion of contaminants in the atmosphere we should study physics that describes the transport of these contaminants in the atmosphere in different boundary conditions. Logan (2001), Mazaher et al. (2013), Scott and Gerhard (2005), Essa et al. (2014) and Tirabassi et al. (2010) studied advection-diffusion equation which depends on Gaussian and non-Gaussian solutions.

Amruta and Pradhan (2013) solved advection-diffusion equation under various circumstances and using various methods.

In this work we solved the advection-diffusion equation in two dimensions to obtain normalized integrated crosswind concentration using Laplace technique. Two models of the vertical eddy diffusivity were developed, considering constant wind speed. One of them depends on downwind distance and the other depends on vertical distance.

Comparisons between them, Gaussian, previous work (Sharan and Modani, 2006) and observed data measured at Copenhagen, Denmark were carried out (Gryning and Lyck, 1984, Gryning et al. 1987).

2. Mathematical models

Diffusion equation is the most important in studying of pollutants dispersion into the atmosphere by using the gradient transport theory, this diffusion equation of pollutants in air can be written as (Tiziano and Vilhena, 2012, Tirabassi et al., 2008, 2009):

\[
\frac{\partial \delta c(x,y,z)}{\partial x} = \frac{k_y}{\frac{\partial y}{\partial y}} \left( k_z \frac{\partial c}{\partial y} \right) + \frac{k_y}{\frac{\partial y}{\partial z}} \left( k_z \frac{\partial c}{\partial z} \right)
\]

where \( u \) is the wind speed (m/s), \( c(x,y,z) \) is the concentration of pollutant (g/m\(^3\)), \( K_y \), \( K_z \) are the eddy diffusivities in lateral and vertical direction respectively.

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2.1. First model

In this model, one supposes that the vertical eddy diffusivity is a function of downwind distance i.e. \( k_y = k(x) \). Integrating equation (1) with respect to \( y \) from \(-\infty\) to \( z \), then:

\[
\frac{\partial c}{\partial y} \int_{-\infty}^{y} c(x,y,z)\,dy = k_y \frac{\partial c}{\partial x}[c(x,y,z)] + \frac{k(x)}{\partial z^2} \int_{-\infty}^{z} c(x,y,z)\,dy
\]  
(2)

By substituting that:

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

One gets that:

\[
k_y \frac{\partial c_y(x,z)}{\partial x} \bigg|_{-\infty}^{z} = 0
\]

By substituting from Eqs. (3) and (4) into Eq. (2), one gets:

\[
\frac{\partial c_y(x,z)}{\partial x} = \frac{k(x)}{\partial z^2} \left[ k(x) \frac{\partial c_y(x,z)}{\partial z} \right]
\]

In first case the eddy diffusivity is supposed to be constant as a function of \( x \).

\[
\frac{\partial c_y(x,z)}{\partial x} = k(x) \frac{\partial c_y(x,z)}{\partial z^2}
\]

Eq. (6) is solved under the boundary conditions:

(i) \( c_y(0,z) = \frac{\partial \delta(z-h_i)}{\partial x} \), where \( h_i \) is a stack height

(ii) \( c_y(x,z) = 0 \) at \( x = \infty \)

(iii) \( k \frac{\partial c_y(x,z)}{\partial x} \bigg|_{z} = 0 \)

where \( z \) is the mixing height.

Taking \( k(x) = \alpha \alpha_x \), where \( \alpha \) is the turbulence parameter such that:

\[
\alpha = \alpha_x, c_v = \text{is the vertical velocity standard deviation (Moreira et al., 2014; Essa et al., 2007; Torber, 2012, Pramod and Sharman, 2016).}
\]

\[
\therefore \ k(x) = \alpha \alpha_x \]

Taking Laplace transform on \( x \) as follows:

\[
\tilde{c}(s,z) = \int_{0}^{\infty} c_y(x,z)e^{-sx}dx
\]

Eq. (6) becomes:

\[
\int_{0}^{\infty} \frac{\partial \tilde{c}}{\partial x} e^{-sx}dx = \int_{0}^{\infty} \frac{\alpha \alpha_x}{\partial z^2} \frac{\partial \tilde{c}}{\partial z} e^{-sx}dx
\]

Integrating Eq. (8), one gets:

\[
-uec_y(0,z) + suc_y(s,z) = \frac{\alpha \alpha_x}{\partial z^2} \frac{\partial \tilde{c}}{\partial z}
\]

Condition (i) is applied in Eq. (9) then:

\[
\frac{\alpha \alpha_x}{\partial z^2} \frac{\partial \tilde{c}}{\partial z} - suc_y(s,z) = -Q \delta(z-h_i)
\]

Now applying Laplace transform on \( z \) one gets:

\[
\int_{0}^{\infty} e^{-s\tilde{c}} \frac{\alpha \alpha_x}{\partial z^2} \frac{\partial \tilde{c}}{\partial z} \,dz - \int_{0}^{\infty} suc^{2}e^{-s\tilde{c}},(s,z)\,dz = -\int_{0}^{\infty} e^{-s\delta}(z-h_i)\,dz
\]

\[
\frac{\alpha \alpha_x}{\partial z^2} \frac{\partial \tilde{c}}{\partial z} - suc_y(s,z) = -Q \int_{0}^{\infty} e^{-s\delta}(z-h_i)\,dz
\]

(10)

After application the condition (iii), Eq. (12) becomes:

\[
\frac{\alpha \alpha_x}{\partial z^2} \left[ p^2 \tilde{c}_y(s,p) - p \tilde{c}_y(0,p) \right] = -Q e^{-s\delta}
\]

(13)

\[
\tilde{c}_y(0,p) = \frac{\alpha \alpha_x}{\partial z^2} \left[ p^2 \tilde{c}_y(0,p) - p \tilde{c}_y(0,p) \right]
\]

(14)

\[
\tilde{c}_y(0,p) = c_y(0,F(p) - Q e^{-s\delta} G(s,p)
\]

(15)

where \( F(s,p) = \frac{p}{(p^2 - \alpha \alpha_x)} \) and \( G(s,p) = \frac{\alpha \alpha_x}{(p^2 - \alpha \alpha_x)} \)

Take the inverse of Laplace transform on “\( z \)” i.e. \( z^{-1}(\tilde{c}_y(s,p)) = c_y(z,s) \)

\[
c_y(z,s) = \frac{c_y(0,p)}{2} \left[ e^{w_{0}} + e^{-w_{0}} \right] - \frac{\alpha \alpha_x}{2} \left[ e^{w_{0}}(z-h_i) - e^{-w_{0}}(z-h_i) \right] H(z-h_i)
\]

(16)

where \( H \) is a Heaviside function.

Let \( R = \frac{h_i}{a} \)

\[
c_y(z,s) = \frac{c_y(0,p)}{2} \left[ e^{w_{0}} + e^{-w_{0}} \right] - \frac{\alpha \alpha_x}{2} \left[ e^{w_{0}}(z-h_i) - e^{-w_{0}}(z-h_i) \right] H(z-h_i)
\]

(17)

\[
c_y(z,s) = c_y(0,s)\cosh(Ra(z-h_i)) - \frac{Q}{Ra} \sinh(Ra(z-h_i)) H(z-h_i)
\]

(18)

Using the boundary condition (iii) one gets:

\[
\frac{\partial \tilde{c}}{\partial z} = R_c c_y(0,s)\sinh(Ra(z-h_i)) - \frac{Q}{Ra} \sinh(Ra(z-h_i)) H(z-h_i)
\]

(19)

\[
c_y(0,s)\sinh(Ra(z-h_i)) = \frac{Q}{Ra} \cosh(Ra(z-h_i)) H(z-h_i)
\]

(20)

\[
c_y(s) = \frac{Q \cosh(Ra(z-h_i))}{Ra} \sinh(Ra(z-h_i))
\]

\[
\therefore c_y(0,s) = \frac{Q \cosh(w_{0}(z-h_i))}{\sinh(w_{0})}
\]

(21)

At ground level (i.e. \( z = 0 \)), \( H(z-h_i) = 0 \), the crosswind integrated concentration can be written as follows:

\[
\tilde{c}_y(z,s) = \frac{Q \cosh(w_{0}(z-h_i))}{\sinh(w_{0})} \frac{\cosh(w_{0})}{\sinh(w_{0})} H(z-h_i)
\]

(22)

2.2. Second Model

In the second model the eddy diffusivity is influenced by the vertical height (\( z \)), and then Eq. (6) can be written as:
\[ \frac{\partial c_n(x,z)}{\partial x} = k_n(z) \frac{\partial^2 c_n(x,z)}{\partial z^2} \]  

Advection–diffusion equation for non-homogeneous turbulence can be solved according to the dependence of eddy diffusivity \( k \) and wind speed profile \( u \) on the height variable \( z \). Therefore, to solve this problem by the Laplace transform technique, a stepwise approximation have been performed of these coefficients discretizing the height \( z_i \) of the PBL into \( N \) sub-intervals in a manner of inside each sub-region, \( k(z) \) and \( u(z) \), assuming the following average values:

\[ k_n = \frac{1}{z_{ni+1} - z_{ni}} \int_{z_{ni}}^{z_{ni+1}} k_n(z) \, dz \]
\[ u_n = \frac{1}{z_{ni+1} - z_{ni}} \int_{z_{ni}}^{z_{ni+1}} u(z) \, dz \]

for \( n = 1:N \).

Applying the Laplace transform on \( x \) under the boundary condition:

1. \( c_n(0,z_{ni}) = \frac{Q}{k_n} \delta (z_{ni} - h_i) \)
2. \( k_n(z) \delta k_n(z_{ni}) = 0 \) at \( z_{ni} = 0, z_i \)

Then the Eq. (23) can be written as:

\[ \int_0^\infty \frac{\partial^2 c_n(x,z)}{\partial z^2} \, dx = k_n \int_0^\infty \frac{\partial^2 c_n(x,z)}{\partial z^2} \, dx \]

Integrating and substituting in the Eq. (25), one gets:

\[ -uc_n(0,z) + sc_n(z) = k_n(z) \frac{\partial^2 c_n(s,z)}{\partial z^2} \]  

Applying the boundary condition (a) one gets:

\[ \frac{\partial^2 c_n(s,z)}{\partial z^2} = \frac{Q}{k_n} \delta (z_{ni} - h_i) \]

Now applying Laplace transform on \( z \) then:

\[ P^{\infty}_{\infty} c_n(s,p) - P^0 c_n (s,0) - \frac{uc_n(s,z)}{k_n} \tilde{c}_n(s,p) = \frac{Q}{k_n} e^{-ph_i} \]

Substituting the condition (b), Eq. (28) becomes:

\[ \frac{\tilde{c}_n(s,p)}{Q} = \frac{c_n(s,0,p)}{p^2 - \frac{\rho}{\mu} (\frac{\rho}{\mu} - \frac{\rho}{\mu})} \]

\[ \frac{\tilde{c}_n(s,p)}{Q} = \frac{c_n(s,0,p)}{p^2 - \frac{\rho}{\mu} (\frac{\rho}{\mu} - \frac{\rho}{\mu})} F(s,p) + \frac{Q}{k_n} e^{-ph_i} G(s,p) \]

where \( F(s,p) = \frac{p}{(p^2 - \frac{\rho}{\mu})} \) and \( G(s,p) = \frac{1}{(p^2 - \frac{\rho}{\mu})} \)

Taking the inverse of Laplace transform on "\( z \)"

i.e. \( L^{-1}(\tilde{f}(s,p),z) = \tilde{c}_n(s,z) \)

\[ \tilde{c}_n(s,z) = \frac{c_n(s,0)}{2} \left[ e^{\frac{\mu}{\rho}} + e^{-\frac{\mu}{\rho}} \right] - \frac{Q}{2k_n} \left[ e^{\frac{\mu}{\rho}} H(z_{ni} - h_i) - e^{-\frac{\mu}{\rho}} H(z_{ni} - h_i) \right] \]

Let \( R_a = \frac{\mu}{\rho} \) and \( R_s = \sqrt{k_n} \)

\[ \tilde{c}_n(s,z) = \frac{c_n(s,0)}{2} \left[ e^{\frac{\mu}{\rho}} + e^{-\frac{\mu}{\rho}} \right] - \frac{Q}{2R_a} \left[ e^{\frac{\mu}{\rho}} H(z_{ni} - h_i) - e^{-\frac{\mu}{\rho}} H(z_{ni} - h_i) \right] \]

\[ \tilde{c}_n(s,z) = \frac{c_n(s,0) \cosh R_a z - Q}{R_a} \sinh R_a (z_{ni} - h_i) H(z_{ni} - h_i) \]

Applying the boundary condition (b) one gets:

\[ \frac{\partial \tilde{c}_n(s,z)}{\partial z_i} = 0 \) at \( z_i = z_i \): then,

\[ \frac{\partial \tilde{c}_n(s,z)}{\partial z_i} = R_c c_n(s,0) \sinh R_a z - \frac{Q}{R_a} \cosh R_a (z_{ni} - h_i) H(z_{ni} - h_i) \]

\[ \frac{Q}{R_a} \sinh R_a (z_{ni} - h_i) \frac{\delta}{\partial z_i} H(z_{ni} - h_i) \]

Comparisons between predicted and observed results were carried out using statistical method (Hanna, 1989). The standard statistical measures that characterize the agreement between prediction \( C_{pr} = C_{pred}/Q \) and observations \( C_{ob} = C_{obs}/Q \):

\[ C_{cn} = \frac{Q}{R_a} \sinh R_a (z_{ni} - h_i) H(z_{ni} - h_i) \]

\[ C_{cn} = \frac{Q}{R_a} c_n(s,0) \sinh R_a z - \frac{Q}{R_a} \cosh R_a (z_{ni} - h_i) H(z_{ni} - h_i) \]

\[ C_{cn} = \frac{Q}{R_a} \cosh R_a (z_{ni} - h_i) H(z_{ni} - h_i) \]
**Table 1**
Comparison between predicted and observed crosswind-integrated normalized concentration with the emission source rate at different boundary layer height, downwind distance, wind speed, scaling convection velocity and distance for different runs.

| Run No. | Date       | PG Stability | $z_0$ (m) | $u^*$(m/s) | $U_{10}$(m/s) | Distance (m) | $C_y/Q$ $(10^{-4} \text{ sm}^{-2})$ | Model assessment |
|---------|------------|--------------|-----------|-------------|---------------|--------------|-------------------------------|----------------|
| 1       | 20-9-78    | A            | 1980      | 0.83        | 2.1           | 1900         | 6.48 | 0.64 | 0.74 | 0.46 | 1.06 | 1.06 |
| 2       | 20-9-78    | A            | 1980      | 0.83        | 2.1           | 3700         | 2.31 | 0.55 | 1.57 | 0.33 | 0.45 | 2.52 |
| 3       | 26-9-78    | C            | 1920      | 1.07        | 4.9           | 2100         | 5.38 | 1.04 | 3.64 | 3.18 | 2.29 |
| 4       | 26-9-78    | C            | 1920      | 1.07        | 4.9           | 4200         | 2.95 | 2.9  | 4.12 | 1.58 | 1.18 |
| 5       | 19-10-78   | B            | 1120      | 0.68        | 2.4           | 1900         | 8.20 | 2.03 | 8.09 | 5.66 | 4.51 |
| 6       | 19-10-78   | B            | 1120      | 0.68        | 2.4           | 3700         | 6.22 | 3.91 | 4.03 | 2.88 | 2.65 |
| 7       | 19-10-78   | B            | 1120      | 0.68        | 2.4           | 5400         | 4.30 | 3.91 | 7.82 | 2.21 | 2.58 |
| 8       | 9-11-78    | C            | 820       | 0.71        | 3.1           | 2100         | 6.72 | 1.25 | 5.02 | 4.81 | 3.63 |
| 9       | 9-11-78    | C            | 820       | 0.71        | 3.1           | 4200         | 5.84 | 3.08 | 6.19 | 2.43 | 2.44 |
| 10      | 9-11-78    | C            | 820       | 0.71        | 3.1           | 6100         | 4.97 | 3.22 | 6.51 | 2.00 | 2.41 |
| 11      | 30-4-78    | C            | 1300      | 1.33        | 7.2           | 2000         | 3.96 | 0.37 | 2.27 | 2.63 | 1.63 |
| 12      | 30-4-78    | C            | 1300      | 1.33        | 7.2           | 4200         | 2.22 | 2.19 | 2.74 | 1.28 | 0.82 |
| 13      | 30-4-78    | C            | 1300      | 1.33        | 7.2           | 5900         | 1.83 | 2.52 | 2.82 | 0.90 | 0.68 |
| 14      | 27-6-78    | B            | 1850      | 0.87        | 4.1           | 2000         | 6.70 | 0.78 | 4.71 | 4.16 | 2.51 |
| 15      | 27-6-78    | B            | 1850      | 0.87        | 4.1           | 4100         | 3.25 | 2.72 | 2.58 | 2.03 | 1.17 |
| 16      | 27-6-78    | B            | 1850      | 0.87        | 4.1           | 5300         | 2.23 | 2.97 | 2.66 | 1.56 | 0.79 |
| 17      | 6-7-78     | D            | 810       | 0.72        | 4.2           | 1900         | 4.16 | 0.16 | 4.61 | 4.87 | 4.20 |
| 18      | 6-7-78     | D            | 810       | 0.72        | 4.2           | 3600         | 2.02 | 1.57 | 2.0  | 2.74 | 2.80 |
| 19      | 6-7-78     | D            | 810       | 0.72        | 4.2           | 5300         | 1.52 | 2.25 | 2.12 | 1.84 | 2.18 |
| 20      | 19-7-78    | C            | 2090      | 0.98        | 5.1           | 2100         | 4.58 | 0.58 | 3.49 | 3.44 | 2.20 |
| 21      | 19-7-78    | C            | 2090      | 0.98        | 5.1           | 4200         | 3.11 | 2.35 | 3.96 | 1.74 | 1.13 |
| 22      | 19-7-78    | C            | 2090      | 0.98        | 5.1           | 6000         | 2.59 | 2.69 | 1.83 | 1.19 | 0.81 |

* Sharan and Modani (2006).

**Table 2**
Comparison between predicted (1), predicted (2), Sharan and Gaussian models according to standard statistical Performance measure.

| Models         | NMSE  | FB     | COR   | FAC2  |
|----------------|-------|--------|-------|-------|
| Predicted 1    | 0.94  | 0.55   | -0.01 | 0.72  |
| Predicted 2    | 0.13  | 0.00   | 0.72  | 1.03  |
| Previous work* | 0.30  | 0.42   | 0.80  | 0.69  |
| Gaussian model | 0.56  | 0.58   | 0.69  | 0.59  |

* Sharan and Modani (2006).

Correlation Coefficient(COR) = $1/\text{N}_{\text{obs}} \sum_{i=1}^{\text{N}_{\text{obs}}} (C_y-C_y^p) \times (C_y-C_y^o)/(\sigma_y \sigma_o)$

Factor of Two(FAC2) = $0.5 \leq \frac{C_y^2}{C_o^2} \leq 2.0$

where $\sigma_y$ and $\sigma_o$ are the standard deviations of predicted $C_y^p$ and observed $C_y^o$ normalized crosswind integrated concentration respectively. Over bars indicate the average over all measurements. For a perfect model NMSE must be = FB = 0 and COR = FAC2 = 1.

5. Conclusions

The predicted models (1 & 2) normalized crosswind integrated concentration of air pollutants was obtained by solving diffusion equation in two dimensions using Laplace technique then, using Gaussian quadrature formulas. Considering that the eddy diffusivity is a function in downwind distance (proposed 1) and depends on the vertical distance (predicted 2) in unstable case. One finds that there is a good agreement between predicted model (2) and the observed concentrations than predicted (1), Gaussian and previous work (Sharan and Modani, 2006).

From the statistical method, one finds that all models are inside a factor of two with observed data. Regarding to NMSE and FB, predicted model (2) is performance well with observed data than predicted (1), the Gaussian and Sharan models in unstable condition. One can conclude that, our predicted model (2) is performance well with the observed concentrations than predicted (1), the previous work (Sharan and Modani, 2006).
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