Calculation of crosswind integrated concentration by using different dispersion schemes

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ABSTRACT. The Gaussian model is the most extensively used model for local dispersion. The Gaussian formula for a continuous release from a point source (GPM) is integrated to get crosswind integrated concentration. Different schemes such as Irwin, power law, Briggs, Standard method, and split sigma theta method can be used to obtain integrated concentration. Also downwind speed in power law, plume rise and Statistical measures are used in the model to know which is the best scheme agrees with the observed concentration data obtained from Copenhagen, Denmark.

Key words – Crosswind integrated concentration, Different schemes, Plume rise, Statistical measures.

1. Introduction

Conventional Gaussian plume models are commonly used for the air quality analysis and regulatory purposes. These Gaussian models are based on the solution of an advection diffusion equation derived by assuming that the wind speed and eddy diffusivity don't have spatial and temporal variations (Haman et al., 1982).

For the practical applications of the solutions obtained, the eddy diffusivities are expressed as functions of downwind distance and wind speed is parameterized as a power law function of the vertical height above the ground (Irwin, 1979).

The commonly used power law approximations for the profiles of wind velocity and vertical diffusivity have been employed to derive analytical solutions (Roa, 1981; Koch 1989; Chitgopekar et al. 1990, Essa et al. 2008 and Sharan and Kumar 2009).

In this work, a Gaussian plume model using different dispersion schemes, wind speed in power law, and plume rise are used to get the crosswind integrated concentrations. Statistical technique is used to compare between the observed and all predicted concentrations obtained from different dispersion schemes to know the best predicted model.

2. Description technique

The Gaussian plume model is still the basic and most common model used for dispersion calculations. It was derived by Sutton (1953), Csanady (1973), Smith (1973), and Turner (1970). The following formula represents the
TABLE 1

Estimates of the power (p) in urban areas for six stability classes based on information by Irwin (1979b)

| Stability Classes       | Very unstable (A) | Moderately unstable (B) | Slightly unstable (C) | Neutral (D) | Slightly stable (E) | Moderately stable (F) |
|-------------------------|-------------------|-------------------------|-----------------------|-------------|--------------------|-----------------------|
| Urban p p               | 0.15              | 0.15                    | 0.20                  | 0.25        | 0.40               | 0.60                  |

concentration of a pollutant releasing from a continuous point source;

\[
C(x, y, z, H) = \frac{Q}{2\pi\sigma_y \sigma_z U} e^{-\frac{y^2}{2\sigma_y^2}} \left[ e^{\frac{(z-H)^2}{2\sigma_z^2}} + e^{\frac{(z+H)^2}{2\sigma_z^2}} \right]
\]

(2.1)

where,

- \( C \) is the concentration of the pollutant at a point with coordinates \( x, y, z \) (g/m³),
- \( x \) is the downwind distance from the source (m),
- \( y \) is the lateral distance from the source (m),
- \( z \) is the vertical distance above the ground (m),
- \( Q \) is the emission rate (g/s),
- \( U \) is the downwind velocity (m/s),
- \( H \) is the effective source height above the ground (m), which is generally presented in the form \( H = h_s + \Delta h \)

where, \( h_s \) is the physical stack height, and \( \Delta h \) is the plume rise.

Finally, \( \sigma_y \) and \( \sigma_z \) are the plume dispersion parameters in the horizontal and vertical directions respectively.

By integrating both sides with respect to \( y \), we can get;

\[
C_y(x, z, H) = \frac{Q}{2\pi\sigma_y \sigma_z U} \left[ e^{\frac{(z-H)^2}{2\sigma_z^2}} + e^{\frac{(z+H)^2}{2\sigma_z^2}} \right] \int_{-\infty}^{\infty} e^{-\frac{y^2}{2\sigma_y^2}} dy
\]

(2.2)

Where \( C_y \) is the crosswind integrated concentration and the dispersion parameters \( \sigma_y \) and \( \sigma_z \) can be calculated using different schemes, here calculating them by five different methods namely, Irwin scheme, Power-Law, Briggs’ scheme, Standard method, and Split sigma theta method.

We can obtain downwind speed \( U_{115} \) at height 115m as follows:

\[
U_{115} = U_{10} \left( \frac{h_s}{10} \right)^p
\]

(2.3)

Where,

- \( U_{115} \) is the wind speed at 115m height.
- \( U_{10} \) is the wind speed at 10m height.
- \( h_s \) is the physical stack height (115m).
- \( p \) is a parameter estimated by Irwin (1979), which is related to stability classes, is given in Table 1.

Also the effective height \( H \) is gotten by Briggs (1969),

\[
H = h_s + \Delta h
\]

(2.4)

\[
\Delta h = 3 \left( \frac{w}{U_{115}} \right) D
\]

(2.5)

Where,

- \( H \) is the effective source height above the ground (m).
- \( h_s \) is the physical stack height (115m).
- \( \Delta h \) is the plume rise (m).
TABLE 2
Values of wind speed at 10 m and 115 m and downwind distance through unstable and neutral stabilities in northern part of Copenhagen

| Run No. | Stability              | U_{10}(m.sec^{-1}) | U_{115}(m.sec^{-1}) | Downwind distance (m) |
|---------|------------------------|---------------------|---------------------|-----------------------|
| 1       | Very unstable (A)      | 2.1                 | 3.029172            | 1900                  |
| 1       | Very unstable (A)      | 2.1                 | 3.029172            | 3700                  |
| 2       | Slightly unstable (C)  | 4.9                 | 7.986117            | 2100                  |
| 2       | Slightly unstable (C)  | 4.9                 | 7.986117            | 4200                  |
| 3       | Moderately unstable (B)| 2.4                 | 3.461911            | 1900                  |
| 3       | Moderately unstable (B)| 2.4                 | 3.461911            | 3700                  |
| 3       | Moderately unstable (B)| 2.4                 | 3.461911            | 5400                  |
| 4       | Slightly unstable (C)  | 2.5                 | 4.074549            | 4000                  |
| 5       | Slightly unstable (C)  | 3.1                 | 5.052441            | 2100                  |
| 5       | Slightly unstable (C)  | 3.1                 | 5.052441            | 4200                  |
| 5       | Slightly unstable (C)  | 3.1                 | 5.052441            | 6100                  |
| 6       | Slightly unstable (C)  | 7.2                 | 11.7347             | 2000                  |
| 6       | Slightly unstable (C)  | 7.2                 | 11.7347             | 4200                  |
| 6       | Slightly unstable (C)  | 7.2                 | 11.7347             | 5900                  |
| 7       | Moderately unstable (B)| 4.1                 | 5.914098            | 2000                  |
| 7       | Moderately unstable (B)| 4.1                 | 5.914098            | 4100                  |
| 7       | Moderately unstable (B)| 4.1                 | 5.914098            | 5300                  |
| 8       | Neutral (D)            | 4.2                 | 7.734349            | 1900                  |
| 8       | Neutral (D)            | 4.2                 | 7.734349            | 3600                  |
| 8       | Neutral (D)            | 4.2                 | 7.734349            | 5300                  |
| 9       | Slightly unstable (C)  | 5.1                 | 8.312081            | 2100                  |
| 9       | Slightly unstable (C)  | 5.1                 | 8.312081            | 4200                  |
| 9       | Slightly unstable (C)  | 5.1                 | 8.312081            | 6000                  |

\( w \) is the exits velocity (4m/s).

\( D \) is the internal stack diameter (1m).

The used data set was observed from the atmospheric diffusion experiments conducted at the northern part of Copenhagen, Denmark, under unstable conditions (Gryning and Lyck, 1984; Gryning et al., 1987). The tracer sulfur hexafluoride (SF\(_6\)) was released from a tower at a height of 115m without buoyancy. The values of different parameters such as stability, wind speed at 10m (\( U_{10} \)), wind speed at 115m (\( U_{115} \)), and downwind distance during the experiment are represented in Table 2.

3. Dispersion parameters schemes

Since the Gaussian plume model is expressed in terms of the dispersion parameters \( \sigma_y \) and \( \sigma_z \), the appropriate selection of horizontal and vertical dispersion parameters is much targeted. We select five different methods namely, Irwin, Power-Law, Brigg’s, Standard, and Split sigma theta methods, for calculating \( \sigma_y \) and \( \sigma_z \) to choose the most accurate one.
3.1. Irwin method

Irwin (1983) proposed the standard deviations of the horizontal and vertical crosswind concentration distribution of pollutant \( \sigma_y \) and \( \sigma_z \) respectively, as follows:

\[
\sigma_y(x) = \sigma_y f_y, \quad \text{and} \quad \sigma_z(x) = \sigma_z f_z,
\]

where,

\[
t = \frac{x}{U_{115}}
\]

for unstable and stable conditions.

\[
f_y = \frac{1}{1 + 0.9 \left( \frac{t}{1000} \right)}, \quad \text{for unstable condition, and} \quad \]

\[
f_z = \frac{1}{1 + 0.9 \left( \frac{t}{50} \right)}, \quad \text{for stable condition.}
\]

\( \sigma_y \) and \( \sigma_z \) are non-dimensional function of travel time and are given by Irwin (1983) as,

\[
\sigma_y = \sigma_w U_{115},
\]

where \( \sigma_w \) and \( \sigma_y \) are the standard deviations of the wind direction in the horizontal and vertical, respectively. Specifications of \( \sigma_w \) and \( \sigma_y \) can be found in Gifford (1976) and Hanna et al. (1982). Based on the Pasquill stability classes from A to F, they are given in Table 3.

So the values \( \sigma_y \) and \( \sigma_z \) are obtained by the following equations,

\[
\sigma_y(x) = \frac{\sigma_w x}{1 + 0.9 \left( \frac{x}{1000U_{115}} \right)}
\]

for stable and unstable conditions,

\[
\sigma_z(x) = \sigma_w x \quad \text{for unstable condition, and} \quad \]

\[
\sigma_z(x) = \frac{\sigma_w x}{1 + 0.9 \left( \frac{x}{50U_{115}} \right)} \quad \text{for stable condition.}
\]

The final results of normalized crosswind-integrated concentration \( C_y/Q \times 10^4 \text{ sm}^{-2} \), after calculating \( \sigma_y \) and \( \sigma_z \) by using Irwin method, are presented in Table 8.

3.2. Power-Law method

Smith (1968) worked out analytical Power-Law formulae for \( \sigma_y \) and \( \sigma_z \) to be uses easily than using a graph or a table. He used the Brookhaven National Laboratory (BNL) formulas, which are defined by him using wind direction \( \theta \) recorded over one hour as follows:

\[
A: \quad \text{fluctuations of } \theta \text{ exceed } 90^\circ. \quad \text{(Very Unstable conditions)}
\]
### TABLE 4
Brookhaven National Laboratory Parameters

| Stability Classes | Moderately unstable (B₁) | Slightly unstable (B₂) | Neutral (D) | Moderately stable (F) |
|-------------------|--------------------------|------------------------|-------------|-----------------------|
| a                 | 0.36                     | 0.40                   | 0.32        | 0.31                  |
| b                 | 0.86                     | 0.91                   | 0.78        | 0.71                  |
| c                 | 0.33                     | 0.41                   | 0.22        | 0.06                  |
| d                 | 0.86                     | 0.91                   | 0.78        | 0.71                  |

### TABLE 5
Formulas produced by Briggs (1973) for $\sigma_y(x)$ and $\sigma_z(x)$ ($102 < x < 104$ m)

| Stability classes | Very unstable (A) | Moderately unstable (B) | Slightly unstable (C) | Neutral (D) | Slightly stable (E) | Moderately stable (F) |
|-------------------|-------------------|-------------------------|-----------------------|-------------|---------------------|------------------------|
| $\sigma_y(x)$     | $0.32x(1+0.0004x)^{1/2}$ | $0.32x(1+0.0004x)^{1/2}$ | $0.22x(1+0.0004x)^{1/2}$ | $0.16x(1+0.0004x)^{1/2}$ | $0.11x(1+0.0004x)^{1/2}$ | $0.11x(1+0.0004x)^{1/2}$ |
| $\sigma_z(x)$     | $0.24x(1+0.001x)^{1/2}$ | $0.24x(1+0.001x)^{1/2}$ | $0.20x$ | $0.14x(1+0.0003x)^{1/2}$ | $0.08x(1+0.00015x)^{1/2}$ | $0.08x(1+0.00015x)^{1/2}$ |

### TABLE 6
Values of the dispersion parameters for the Pasquill stability classes

| Stability classes | Very unstable (A) | Moderately unstable (B) | Slightly unstable (C) | Neutral (D) | Slightly stable (E) | Moderately stable (F) |
|-------------------|-------------------|-------------------------|-----------------------|-------------|---------------------|------------------------|
| r                 | 250               | 202                     | 134                   | 78.7        | 56.6                | 37                     |
| s                 | 102               | 96.2                    | 72.2                  | 47.5        | 33.5                | 22                     |
| A                 | 0.927             | 0.370                   | 0.283                 | 0.707       | 1.07                | 1.17                   |
| P                 | 0.189             | 0.162                   | 0.134                 | 0.135       | 0.137               | 0.134                  |
| q                 | -1.918            | -0.101                  | 0.102                 | 0.465       | 0.624               | 0.70                   |

### TABLE 7
Values of wind direction fluctuations in the lateral direction $\sigma_\theta$ for the Pasquill stability classes

| Stability classes | Very unstable (A) | Moderately unstable (B) | Slightly unstable (C) | Neutral (D) | Slightly stable (E) | Moderately stable (F) |
|-------------------|-------------------|-------------------------|-----------------------|-------------|---------------------|------------------------|
| $\sigma_\theta$   | $25^\circ$        | $20^\circ$              | $15^\circ$            | $10^\circ$  | $5^\circ$           | $2.5^\circ$            |
**TABLE 8**

The comparison between observed, at ground in diffusion experiment in northern part of Copenhagen, and different calculated crosswind-integrated concentrations $C_y/Q \times 10^{-4}$ (sm$^{-2}$) obtained from the used dispersion schemes

| Distance (x) (m) | Stability | Observed (C/Q) | Calculated Gaussian (C/Q) | Calculated Irwin (C/Q) | Calculated Power-Law (C/Q) | Calculated Briggs (C/Q) | Calculated Standard (C/Q) | Calculated Standard (C/Q) |
|-----------------|-----------|----------------|--------------------------|-----------------------|---------------------------|-------------------------|--------------------------|--------------------------|
| 1900            | A         | 6.48           | 5.16                     | 0.1386                | 10.4147                   | 8.9125                  | 6.0404E-09               | 6.04036E-09              |
| 3700            | A         | 2.31           | 2.52                     | 0.0712                | 6.4993                    | 6.1651                  | 8.6428E-10               | 8.64269E-10              |
| 2100            | C         | 5.38           | 2.29                     | 7.3191                | 2.2276                    | 2.2890                  | 0.0164                   | 0.0164                   |
| 4200            | C         | 2.95           | 1.18                     | 3.6596                | 1.2168                    | 1.1780                  | 0.0088                   | 0.0088                   |
| 1900            | B         | 8.2            | 4.51                     | 0.1516                | 9.1242                    | 7.8048                  | 0.0053                   | 0.0053                   |
| 3700            | B         | 6.22           | 2.65                     | 0.0779                | 5.6891                    | 5.3963                  | 0.0026                   | 0.0026                   |
| 5400            | B         | 4.3            | 2.58                     | 0.0534                | 4.2034                    | 4.3802                  | 0.0017                   | 0.0017                   |
| 4000            | C         | 11.7           | 6.29                     | 7.5315                | 2.4900                    | 2.4213                  | 0.0180                   | 0.0180                   |
| 2100            | C         | 6.72           | 3.63                     | 11.5689               | 3.5191                    | 3.6160                  | 0.0259                   | 0.0258                   |
| 4200            | C         | 5.84           | 2.44                     | 5.7846                | 1.9230                    | 1.8617                  | 0.0139                   | 0.0139                   |
| 6100            | C         | 4.97           | 2.41                     | 3.9828                | 1.3763                    | 1.2885                  | 0.0099                   | 0.0099                   |
| 2000            | C         | 3.96           | 1.63                     | 5.2300                | 1.5801                    | 1.6298                  | 0.0116                   | 0.0116                   |
| 4200            | C         | 2.22           | 0.82                     | 2.4906                | 0.8281                    | 0.8018                  | 0.0060                   | 0.0060                   |
| 5900            | C         | 1.33           | 0.68                     | 1.7730                | 0.6107                    | 0.5734                  | 0.0044                   | 0.0044                   |
| 2000            | B         | 6.7            | 2.51                     | 0.0843                | 5.1916                    | 4.4528                  | 0.0029                   | 0.0029                   |
| 4100            | B         | 3.25           | 1.17                     | 0.0411                | 3.0751                    | 2.9867                  | 0.0013                   | 0.0013                   |
| 5300            | B         | 2.23           | 0.97                     | 0.0318                | 2.5000                    | 2.5921                  | 0.0010                   | 0.0010                   |
| 1900            | D         | 4.16           | 4.2                      | 0.0987                | 4.4243                    | 4.1796                  | 0.4490                   | 0.3175                   |
| 3600            | D         | 2.02           | 2.8                      | 0.0521                | 5.3033                    | 2.7923                  | 0.3191                   | 0.3191                   |
| 5300            | D         | 1.52           | 2.18                     | 0.0354                | 4.6061                    | 2.1671                  | 0.2595                   | 0.1835                   |
| 2100            | C         | 4.58           | 2.2                      | 7.0320                | 2.1403                    | 2.1993                  | 0.0157                   | 0.0157                   |
| 4200            | C         | 3.11           | 1.13                     | 3.5161                | 1.1690                    | 1.1318                  | 0.0084                   | 0.0084                   |
| 6000            | C         | 2.59           | 0.81                     | 2.4613                | 0.8492                    | 0.7962                  | 0.0061                   | 0.0061                   |

B$_1$ : fluctuations of $\theta$ from 40 to 90°. (Moderately Unstable)

B$_2$ : fluctuations of $\theta$ from 15 to 40°. (Slightly Unstable)

C : fluctuations of $\theta$ greater than 15° with strip chart showing an unbroken solid core in the trace. (Neutral)

D : Trace in a line, short-term fluctuations in $\theta$ less than 15°. (Moderately Stable).
He summarized the BNL formulas which are based on hourly average measurements of diffusion to about 10 km of a nonbuoyant plume released from a height of 108 m:

\[ \sigma_y = ax^b \]

(3.11)

\[ \sigma_z = cx^d \]

(3.12)

Values of the parameters a, b, c, and d are given in Table 4.

Because of the absence of the Very Unstable condition in the solution of Smith (1968), here we use values of the Moderately Unstable condition parameters to calculate cases of the Very Unstable condition. The final results of crosswind-integrated concentration \( C_y/Q \) \((10^4 \text{ sm}^{-2})\), after calculating \( \sigma_y \) and \( \sigma_z \) by using Power-Law method, are presented in Table 8.
### TABLE 9
Comparison between our different models according to standard statistical performance measure

| Models                | NMSE | FB  | COR  | FAC2 |
|-----------------------|------|-----|------|------|
| Gaussian model        | 0.58 | 0.58| 0.80 | 0.60 |
| Irwin method          | 1.07 | 0.48| 0.39 | 0.62 |
| Power-Law method      | 0.59 | 0.24| 0.32 | 0.94 |
| Briggs' method        | 0.66 | 0.42| 0.39 | 0.75 |
| Standard method       | 173.08| 1.97| -0.31| 0.02 |
| Split sigma theta method| 134.35| 1.96| -0.24| 0.02 |

3.3. Briggs method

Briggs (1973) used theoretical concepts of the related formulas to get set of formulas can be used in common practices. According to these formulas $\sigma_y$ and $\sigma_z$ is proportional to $x$ at all stability conditions. Also $\sigma_y$ and $\sigma_z$ are independent of release height and roughness in these formulas. The values of $\sigma_y$ and $\sigma_z$ in urban conditions are given in Table 5.

The final results of crosswind-integrated concentration $C_y/Q\ (10^{-4}\ \text{sm}^{-2})$ after calculating $\sigma_y$ and $\sigma_z$ by using Briggs method are presented in Table 8.

3.4. Standard method

In this method, $\sigma_y$ and $\sigma_z$ can be analytically expressed, based on $(P-G)$ curves, using the following forms:

$$\sigma_y = \frac{rx}{\left(1 + \frac{x}{a}\right)^p}, \text{ and}$$  

$$\sigma_z = \frac{sx}{\left(1 + \frac{x}{a}\right)^q} \quad (3.13) \quad \text{and} \quad (3.14)$$

Where $r$, $s$, $a$, $p$, and $q$ are constants depending on the atmospheric stability. Their values are given in Table 6.

The final results of crosswind-integrated concentration $C_y/Q\ (10^{-4}\ \text{sm}^{-2})$ after calculating $\sigma_y$ and $\sigma_z$ by using Standard method are presented in Table 8.

3.5. Split sigma theta method

Here $\sigma_y$ is estimated as in the Standard method, while $\sigma_z$ is estimated using the wind direction fluctuations in the lateral direction $\sigma_\theta$ in the different stability classes through the following relationship:

$$\sigma_y = x\sinh\left(\sigma_\theta^2\right)$$  

$$(3.15)$$

The values of the wind direction fluctuations in the lateral direction $\sigma_\theta$ in the different stability classes are given in Table 7.

The final results of crosswind-integrated concentration $C_y/Q\ (10^{-4}\ \text{sm}^{-2})$ after calculating $\sigma_y$ and $\sigma_z$ by using Split sigma theta method are presented in Table 8.

4. Comparison between the used methods

In this section, we compare between the final results obtained using the five different schemes. We look for which is the most optimum method to be used. Fig. 1 shows the relation between the observed and calculated crosswind concentrations of the tracer sulfur hexafluoride (SF$_6$) with downwind distances from continuous source.
In this Fig. 1, you can notice that the observed concentrations line is not near by one identified line. So each model has some points near the observed results while the others are not. In the Fig. 2, we plot the normalized crosswind concentrations calculated using different Gaussian models versus the observed concentrations.

Regarding Fig. 2, we can observe that the Standard method and the Split sigma theta method are almost near Zero line. But it stills difficult to know which is the most accurate among Gaussian, Power, Briggs, and Irwin methods.

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 \( C_p = C_{\text{pred}}/Q \) and observations \( C_o = C_{\text{obs}}/Q \):

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

(4.1)

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

(4.2)

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

(4.3)

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

(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:

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

From the statistical method, we find that the Gaussian model, Irwin, power law, Briggs methods are factors of 2 with observed data. Regarding to NMSE, the mentioned methods can be considered as good models except for Irwin which is relatively far. Power-Law method is the best relating to FB, while the Gaussian Model and the Power-Law are the best correlation with observed data. The calculated concentrations using standard and split sigma theta methods are far from the observed concentrations.

5. Conclusions

Gaussian plume models are commonly used for the air quality analysis and regulatory purposes. From the final results, we can conclude that calculated concentrations obtained from Irwin, power law, Briggs as well as Gaussian models are agree with the observed concentrations when the wind speed is greater than 2 m/s. While the calculated concentrations using standard and split sigma theta methods can be acceptable if the wind speed is less than 2 m/s.

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