ACADEMIA ROMÂNĂ
Revue Roumaine de Chimie
https://www.icf.ro/rrch/

Rev. Roum. Chim.,
2024, *69*(1–2), 33–39
DOI: 10.33224/rrch.2024.69.1-2.04

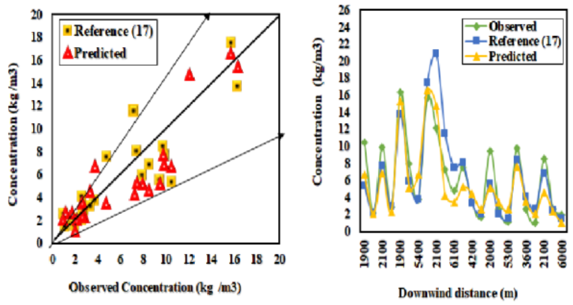
EVALUATION GAUSSIAN CONCENTRATION USING DISPERSION PARAMETERS IN PUFF PLUME MODEL

Khaled S. M. ESSA and Sawsan I. M. ELSAID*

Department of Mathematics and Theoretical Physics, Nuclear Research Center, Egyptian Atomic Energy, Authority, Cairo, Egypt

Received May 31, 2023

The proposed concentrations model was compared to observed data from air diffusion studies for hexafluoride (SF_6) conducted in the northern area of Copenhagen, Denmark, and earlier work for the Gaussian puff model. The predicted concentrations and earlier studies were found to be within a factor of two of each other, indicating that the predicted data is compatible with the observed concentrations data. Under unstable conditions, the statistical statistics show a reasonable agreement between the expected and observed concentrations at the Copenhagen Experimental. In contrast to the previous work's results, which had an NMSE of 0.3 and an FB of 0.21, we discovered that the data obtained using the statistical method had an NMSE of 0.2 and an FB of 0.25. The projected COR is 0.95, compared to 0.97 in a previous computation. The observed concentration data was 88% of the expected value, compared to 78% in previous research. The expected data are consistent with the observed concentration measurements. When compared to previous work, the Copenhagen experiment was conducted under unstable conditions, and statistical data show good agreement between predicted and observed concentrations.



INTRODUCTION

The puff model was used to simulate and predict air dispersion based on a few fundamental assumptions[1]. Parameterization of Gaussian dispersion modifications in various models was used.[2,3] Previous notes were gathered in terms of Pasquill stability.[4]

Its scattering parameters were created using the planetary boundary layer (PBL) perturbation and their capacity to replicate experimental scattering data, primarily for regulatory purposes. Gaussian models are quick and easy to use; the AERMOD was the most widely.[5]

AERMOD was the most famous Gaussian model and one of the inflation models that defines the CALPUFF Plume model, which is not a Gaussian model.[6–10]

Discovered that increasing the number of particles in the PUFF-UAF model, using a scattering model based on the Lagrangian approach, and tracking methods had a substantial impact on the results. However, the PUFF-UAF model predicted ash concentration but failed to accurately depict dispersion.[11]

Presents a basic introduction to air pollution dispersion modelling in layman's terms and covers

* Corresponding author: sawsanibrahim74@yahoo.com

the currently available models. A special emphasis is placed on models and applications that have been cited in the recent five years Gaussian distribution is a good approximation for transient (instantaneously released) puff concentration distributions within a short period after release. Artificial neural network (ANN) models for puff dispersion coefficients were developed.[12]

In this paper, The proposed concentrations model was compared to observed data from air diffusion investigations for hexafluoride (SF_6) conducted in the northern area of Copenhagen, Denmark, and earlier work for the Gaussian puff model.

MATERIALS AND METHODS

Description of the Gaussian Models

The Gaussian Plume

Gaussian models have been frequently utilized for near-scale dispersion modelling since they are based primarily on the smooth analytical formulations for both the Gaussian plume and the Gaussian puff developed.[13]

According to the formula for a Gaussian plume, the concentration is given:

$$\mathbf{C(x,y,z)} = \frac{\mathbf{Q}}{\mathbf{2\pi\sigma_y\,\sigma_z\,u}}\left(\mathbf{Exp}\left(-\frac{\mathbf{(z-h)^2}}{\mathbf{2\sigma_z{}^2}} + \mathbf{Exp}\left(\frac{\mathbf{-(z-h)^2}}{\mathbf{2\sigma_z{}^2}}\right)\right)\right) \tag{1}$$

where C is the concentration of pollutant (g/m^3), x is the downwind distance (m), y is the crosswind distance (m), z is the vertical height (m), Q is the emission rate (g/s), u is the wind speed (m/s), H is the effective height (m), σ_y *and* σ_z are the dispersion parameters in crosswind and vertical height (m).

Puff Models

Puff models have been developed on the Gaussian distribution of the focusing pattern. In contrast, the plume's centerline follows a Lagrangian path rather than a straight line downwind in (Fig. 1).

The concentration was the sum of all puff distributions:

$$\frac{C(x,y,z)}{Q} = \frac{\boldsymbol{\Delta t}}{(2\pi)^{\frac{3}{2}}}\sum_{k=1}^{n}\frac{1}{\sigma_{xk}\sigma_{yk}\sigma_{zk}}\left(exp\left(-\frac{(x_k-x)^2}{2\sigma_{xk}{}^2}-\frac{(y_k-y)^2}{2\sigma_{yk}{}^2}-\frac{(z_k-z)^2}{2\sigma_{zk}{}^2}\right)\right) \tag{2}$$

where Q by the *Ät* is the source term, n is the number of puffs, (x_k, y_k, z_k) are the locations of the k^{th} puff, and deviations from the Gaussian distribution inside the k^{th} puff in the x, y, and z directions, respectively. In a full 3D model, a reflection of the puff's trajectory must also be computed. The plume rise parameterization or a combination of the trajectory and in-puff treatments can be used to quantify the impact of buoyancy. The model can illustrate the source's temporal variability by multiplying the time-dependent source intensity in Q by the puff release frequency. Each puff follows the route specified by the local wind's velocity vector from its centre. Puff models assume that for each pollutant emission in a time interval (t), a mass of pollutants is released into the atmosphere. The model can illustrate the source's temporal variability by multiplying the time-dependent source intensity in Q by the Δt release frequency of puffs. Puff models assume that each pollutant emission in a time interval t releases a mass of pollutants $M = Q\ \Delta t$ into the atmosphere. Each puff has the mass M and is carried by the varying wind in space and time. The assessment of concentration in the diffusion region is affected by wind speed.

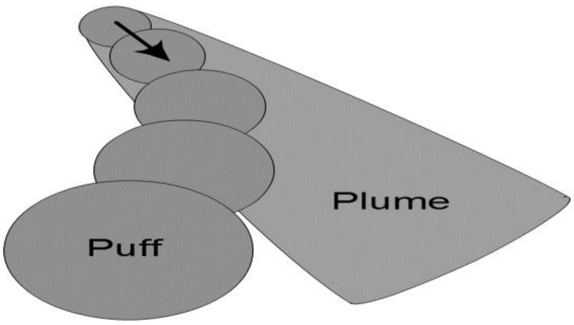


Fig. 1 – Schematic representation of Gaussian plume and puff models. Puff models still estimate a Gaussian dispersion, but can take into account temporal and spatial wind changes.

While each puff is defined as

$$x_0 = \bar{u}\boldsymbol{\Delta}t;\ y_0 = \bar{v}\boldsymbol{\Delta}t;\ and\ z_0 = \bar{w}\boldsymbol{\Delta}t$$

The puffs are emitted at time intervals Δt_1 = 600 s, and the calculation of the concentration of pollutants is made with a time resolution Δt_2= 60s.

The total concentration of a pollutant at a location in space is given by the sum of all puffs.[14]

$$\mathbf{C_T(x,y,z,t)} = \sum_{\text{puffs}}^{\text{total of puffs}} \left[\frac{\Delta M_{puff}}{\left\{\int_{t=0}^{\infty} c_{puff}(x,y,z,t) H(t-t_0)\right\}} \right] \quad (3)$$

H is the Heaviside function, such that $H(t–t_0) = 0$ if $(t–t_0) < 0$ and $H(t–t_0) = 1$ if $(t–t_0) \geq 0$ and:

$$c_{puff}(x,y,z,t) = c_1(x,t)c_2(y,t)c_3(z,t) \quad (4)$$

where c_1, c_2, and c_3 in the Gaussian models are given as follows:

$$c_1 = \frac{1}{\left(\sqrt{2\pi}\right)\sigma_x} \exp\left(-\frac{1}{2}\left(\frac{x-x_0}{\sigma_x}\right)^2\right) \quad (5)$$

$$c_2 = \frac{1}{\left(\sqrt{2\pi}\right)\sigma_y} \exp\left(-\frac{1}{2}\left(\frac{y-y_0}{\sigma_y}\right)^2\right) \quad (6)$$

$$c_3 = \frac{1}{\left(\sqrt{2\pi}\right)\sigma_z} \exp\left(-\frac{1}{2}\left(\frac{z-z_0}{\sigma_z}\right)^2\right) \quad (7)$$

where, σ_x, σ_y, and σ_z are standard diffusion coefficients, The lateral and vertical dispersion parameters constitute the turbulent parameterization and contain the physical components that explain the dispersion process and pollutant plume in the PBL under the influence of turbulent motion.[15]

The algebraic formula for the dispersion parameters is modified as follows.[16]

$$\frac{\sigma_\alpha^2}{z_i^2} = \frac{1.06 c_i \psi^{2/3} \left({}^{z}/_{z_i}\right)^{2/3} (f_m^*)_i^{-2/3} X^2}{1 + \frac{2\sqrt{1.06 c_i}}{\gamma}\left[\psi^{1/3}\left({}^{z}/_{z_i}\right)^{2/3} (f_m^*)_i^{2/3} X\right]} \quad (8)$$

While, σ_x, σ_y and σ_z in the Gaussian models has forms as follows:

$$\sigma_x = z_i \sqrt{\frac{1.06 c_u \psi^{2/3} \left({}^{z}/_{z_i}\right)^{2/3} (f_m^*)_u^{-2/3} X^2}{1 + \frac{2\sqrt{1.06 c_u}}{\gamma}\left[\psi^{1/3}\left({}^{z}/_{z_i}\right)^{2/3} (f_m^*)_u^{2/3} X\right]}}$$

$$\sigma_y = z_i \sqrt{\frac{1.06 c_v \psi^{2/3} \left({}^{z}/_{z_i}\right)^{2/3} (f_m^*)_v^{-2/3} X^2}{1 + \frac{2\sqrt{1.06 c_v}}{\gamma}\left[\psi^{1/3}\left({}^{z}/_{z_i}\right)^{2/3} (f_m^*)_v^{2/3} X\right]}}$$

$$\sigma_z = z_i \sqrt{\frac{1.06 c_w \psi^{2/3} \left({}^{z}/_{z_i}\right)^{2/3} (f_m^*)_w^{-2/3} X^2}{1 + \frac{2\sqrt{1.06 c_w}}{\gamma}\left[\psi^{1/3}\left({}^{z}/_{z_i}\right)^{2/3} (f_m^*)_w^{2/3} X\right]}}$$

where, $\alpha = x, y, z$ are the three components in horizontal, lateral and vertical directions and $i = u, v, w$ are the three components of the velocity in the three directions respectively. $X = \frac{x w_*}{U z_i}$ is a nondimensional distance defined by the ratio of travel time (x/U) to the convective time scale (z_i/w_*), $c_i = \alpha_i \{0.5 \pm 0.05\}(2\pi k)^{-2/3}$ and $\alpha_i = \frac{1{,}4}{\frac{3{,}4}{3}}$ for u, v, w components respectively.[17]

k = 0.4 is von Karman constant ψ =0.65, $(f_m^*)_w = \left({}^{z}/_{z_i}\right)$, $\gamma = \frac{\sqrt{\pi}}{4}$ 17 and $(f_m^*)_v = {}^{z}/_{1.5 z_i}$.[18]

RESULTS AND DISCUSSION

Near Resound, the Copenhagen experimental data set provided observational data for the data used from.[19,20] Sulphur hexafluoride (SF_6) trace concentrations and meteorological measurements were released without buoyancy from a tower at a height of 115 m in the Copenhagen experiment and then collected at locations up to three crosswinds of the detector sampling units, 2–6 km from the point of release. For a total sampling time of one hour, three consecutive concentrations were measured over 20 minutes. With a 0.6 m roughness.

Table 1

Compares the concentration per emission rate under unstable conditions and downwind distance, according to research[16]

Run no.	Stability	Downwind Distance(m)	Concentration /Q (10^{-7} s/m^3)		
			Observed	Reference (16)	Predicted
1	A	1900	10.5	5.34	6.67
1	A	3700	2.14	2.17	2.03
2	B	2100	9.85	7.67	6.85
2	C	4200	2.83	2.93	2.24
3	A	1900	16.33	13.74	15.33
3	D	3700	7.95	5.95	5.14
3	E	5400	3.76	3.72	6.67
5	C	4000	15.71	17.51	16.59
5	A	2100	12.11	20.94	14.73
5	D	4200	7.24	11.49	4.23
6	B	6100	4.75	7.52	3.44
6	A	2000	7.44	8.02	5.22
6	A	4200	3.37	3.24	4.44
7	A	5900	1.74	2.07	2.62
7	A	2000	9.48	5.55	5.15
7	B	4100	2.62	2.03	3.41
8	C	5300	1.15	1.44	2.56
8	A	1900	9.76	8.43	7.66
8	A	3600	2.64	4.06	3.55
9	A	5300	0.98	2.59	2.04
9	B	2100	8.52	6.86	4.52
9	C	4200	2.66	2.55	2.33
9	A	6000	1.98	1.53	0.98

Table 2

The Copenhagen experiment's boundary layer height was described

Run no.	1	2	3	4	5	6	7	8	9
Z_i [m]	1980	1920	1120	390	820	1850	810	2090	1890

Table 3

Shows the convective velocity (w [m/s]) for various runs

Run no.	1	2	3	4	5	6	7	8	9
1	1.17	2.04	1.21	1.32	0.93	1.92	1.93	1.99	1.35
2	2.33	1.85	1.10	1.45	1.10	1.34	1.86	2.27	1.63
3	1.35	2.02	1.40	1.29	0.90	1.22	2.37	2.35	1.77
4	1.22	2.11	1.18	1.37	0.82	1.66	2.15	2.32	1.43
5	1.81	2.15	1.09	1.15	1.05	1.45	1.57	2.42	1.31
6	1.67	1.89	1.37	1.10	1.02	2.34	2.67	2.07	1.47
7	1.98	2.39	1.29	0.89	1.02	1.11	2.37	2.49	1.51
8	2.18	2.26	1.48	0.85	0.89	1.03	2.62	2.35	1.63
9	1.56	2.25	0.92	0.77	0.76	0.88	2.87	2.24	1.74
10	2.29	1.69	1.38	0.77	0.76	0.79	2.15	2.31	1.59
11	1.88	2.28	1.18	0.77	0.76	0.74	1.45	2.54	1.82
12	2.00	1.54	1.37	0.77	0.60	0.65	2.08	2.57	2.03

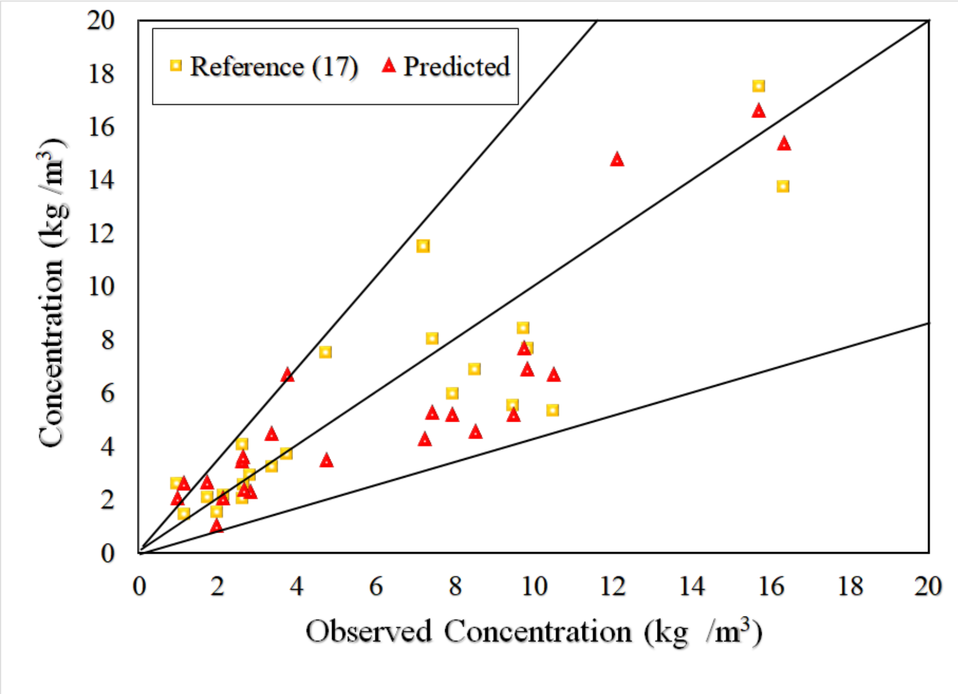


Fig. 2 – Shows the comparison of the observed and predicted concentrations.

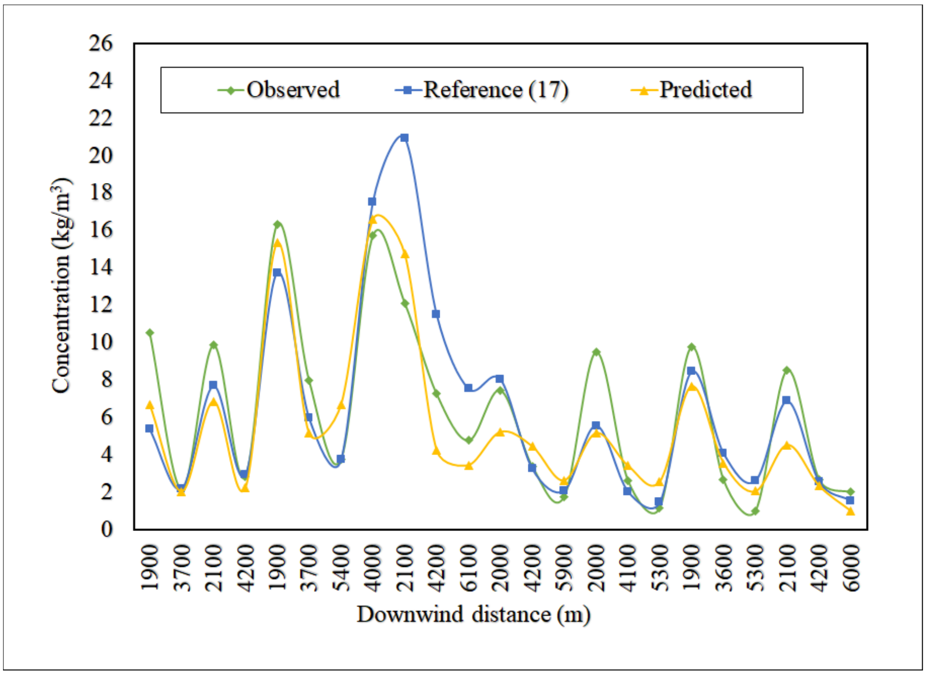


Fig. 3 – Shows the comparison between concentrations and downwind distance.

The relationship between the observed, expected, and reference concentrations is explained in (Table 1) and we discovered that the predicted results are near to observed concentrations and better than the reference. In (Table 2), boundary layer height values (m) are shown. The convective velocity (w [m/s]) for various runs is shown in (Table 3).

One finds the predicted concentrations are within a factor of two of the observed concentrations from previous work as shown in Fig 2. While Fig 3 shows the comparison between concentration per emission rate and downwind distance, the dotted line represents the reference, the dashed line represents the predicted, and the straight line represents the observed.

Model Evaluation Statistics

Use the following statistical techniques to describe the agreement between expected and observed concentrations to assess the model's correctness these measures define: [21]

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

$$\textbf{Normalized Mean Square Error (NMSE)} = \frac{\overline{(C_p - C_o)^2}}{\overline{(C_p C_o)}}$$

$$(C_{pi} - \overline{C_p}) \times \frac{(C_{oi} - \overline{C_o})}{((\sigma_p \sigma_o)]}]$$

$$\textbf{Factor of Two (FAC2)} = 0.5 \le \frac{C_p}{C_o} \le 2.0$$

The factor of Two (FAC2) = $0.5 \le Cp/C_0 \le 2.0$, where σ_p and σ_o are the standard deviations of predicted ($C_p = C_{pred}/Q$) and observed ($C_0 = C_{obs}/Q$) concentrations, respectively. Overbear indicates the average value. The perfect model must have the following characteristics: the normalized mean square error = the fraction bias = 0, and the correlation coefficient = the factor of two = 1.0.

Table 4

Shows a statistical evaluation of the predicted model against the Copenhagen experiment

Models	NMSE	FB	COR	FAC2
Predicted	0.2	0.25	0.95	0.88
Reference (17)	0.3	0.21	0.97	0.78

According to (Table 4) analysis, our results employing the statistical method's NMSE equals 0.2 and FB equals 0.25, while theirs equals 0.3 and FB equals 0.21 when compared to old Reference

The COR was estimated and the Reference study to range between 0.95 to 0.97. By a factor of two, the data and observed data agree. Statistics indicate that there is good agreement between the concentrations reported by Reference (17) and expectations.

CONCLUSIONS

The proposed concentrations model was compared to observed data from air diffusion investigations for hexafluoride (SF6) conducted in the northern area of Copenhagen, Denmark, and earlier work for the Gaussian puff model by Reference (17). The anticipated concentrations and previous study Reference (17) were found to be within a factor of two of each other, suggesting that the predicted data is congruent with the observed concentrations data.

The statistical data demonstrate a fair agreement between the expected and observed concentrations at the Copenhagen Experimental under unstable settings. In contrast to the results of the earlier work, where the NMSE was equal to 0.3 and FB to 0.21, we discovered that the data we acquired using the statistical method have an NMSE of 0.2 and an FB of 0.25. The anticipated COR is 0.95, compared to a prior calculation by Reference (17) that put the COR at 0.97. The observed concentration data was 88% of what was expected, compared to 78% in the earlier studies. The expected data so agree with the concentration data that have been seen. The Copenhagen experiment was conducted under unsteady conditions, and statistical data demonstrate good agreement between predicted and observed concentrations when compared to earlier work by Reference (17).

List of Abbreviations

NMSE – the normalized mean square error
FB – The fraction bias
COR – the correlation coefficient
FAC2 – the factor of two

Acknowledgments. Authors should obtain permission to acknowledge a chief Editor and reviewers in this journal and all members in my department.

REFERENCES

1. T. Mikkelsen S. E. Larsen and I. Troen, I., Risø National Laboratory, **1980**, Risø-M No. 2258.
2. F. Pasquill and F. B. Smith, “Atmospheric diffusion”, 3rd edition, Wiley, Chichester, 1983, p. 297.

3. P. Arya, *J. Appl. Meteorology*, **1995**, *34*, 1112–1122.
4. N. F. Islitzer and D. H. Slade, “Diffusion and transport experiments”, in D. H. Slade (Ed.), “Meteorology and atomic energy”, TID-24190. USAEC, Springfield, 1968, pp. 163–175.
5. D. B. Turner, “Workbook of atmospheric dispersion estimates–an introduction to dispersion modeling”, 2nd edition, CRC, Boca Raton, 1994. p. 192.
6. S. R. Hanna, G. A. Briggs, J. Deardoff, B. A. Egan, F. A. Gifford and F. Pasquill, *Bull. Am. Meteorolog. Soc.*, **1977**, *58*, 1305–1309.
7. G. A. Briggs, *Am. Meteorolog. Society*, **1975**, 59–111.
8. S. R. Hanna, *J. Climate Appl. Meteorolog.*, **1986** , *25*, 1426–1433.
9. K. S. M. Essa and E. A. Fouad, *Australian J. Basic Appl. Sci.*, **2011**, *5*, 1580–1587.
10. A. J. Cimorelli, S. G. Perry, A. Venkatram, J. C. Weil, R. J. Paine, R. B. Wilson, R. F. Lee,W. D. Peters and R. W. Brode, *J. Appl. Meteorolog. Climatolog.*, **2005**, *44*, 682–693. DOI: https://doi.org/10.1175/JAM2227
11. J. S. Scire, D. G. Strimaitisand and R. J. Yamartino, “A User’s Guide for the CALPUFF Dispersion Model”, Version 5, Earth Tech Inc., Lowell, 2000; http://www.src.com/ calpuff /calpuff1.htm
12. L. Jooyong, L. Sungsu, A.-S. Hyun and W.-H. Yi., *Scientifc Reports*., **2021,** *11*, 6456–6462; https://doi.org/10.1038/s41598-021-86039-y
13. J. B. Johnson, *Environ. Sci. Proc.*, **2022**, *19*, 18–24; https://doi.org/10.3390/ecas2022-12826
14. S. Arya, “Air Pollution Meteorology and Dispersion”, Oxford University Press, 1998, p. 310.
15. E. J. Gomes da Silva, T. Tirabased, M. T. Vilbena, D. Buske and R. Sperotte de Quadros, *22nd Int. Congress of Mechanical Engineering November*, **2015**.
16. S. A. Abdul-Wahab, *Eco. Modelling*, **2006**, *197*, 13–20; https://doi.org/10.1016/j.ecolmodel.2006.02.021
17. L. Buligon, G. A. Degrazia, C. R. P. Szinvelski and A. Goulart, *The Open Atmos. Sci. J.*, **2008**, *2*, 153–159; DOI:10.2174/1874282300802010153
18. F. H. Champagne, C. A. Friehe, J. C. Larve and J. C. Wyngaard, *J. Atmos. Soc*., **1977**, *34*, 515–520.
19. S. J. Cauchey and S. G. Palmer, *Q. J. R. Meteorol. Soc.*, **1979**, *105*, 811–827.
20. S. E. Gryning, E. Lyck, *J. Clim. Appl. Meteorol.*, **1984**, *23*, 651–660.
21. S. E. Gryning, A. A. M. Holtslag, J. S. Irwin and B. Sivertsen, *Atmos. Environ*., **1987**, *21*, 79–89.
22. S. R. Hanna, *Atom Environ*., **1989**, *23*, 1385–1395.