

Algebraic Formulation for the Dispersion Parameters in an Unstable Planetary Boundary Layer: Application in the Air Pollution Gaussian Model

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Abstract: An alternative formulation for the dispersion parameters in a convective boundary layer is presented. The development consists of a simple algebraic relation for the dispersion parameters, originated from the fitting of experimental data, in which the turbulent velocity variances and the Lagrangian decorrelation time scales are derived from the turbulent kinetic energy convective spectra. Assuming homogeneous turbulence for elevated regions in an unstable planetary boundary layer (PBL), the present approach, which provides the dispersion parameters, has been compared to the observational data as well as to results obtained by classical complex integral formulations. From this comparison yields that the vertical and lateral dispersion parameters obtained from the simple algebraic formulas reproduce, in an adequate manner, the spread of contaminants released by elevated continuous source in an unstable PBL. Therefore, the agreement with dispersion parameters available by an integral formulation indicates that the hypothesis of using an algebraic formulation as a surrogate for dispersion parameters in the turbulent convective boundary layer is valid. In addition, the algebraic vertical and lateral dispersion parameters were introduced into an air pollution Gaussian diffusion model and validated with the concentration data of Copenhagen experiments. The results of such Gaussian model, incorporating the algebraic dispersion parameters, are shown to agree with the measurements of Copenhagen.

Keywords: Lateral and vertical dispersion parameters, dispersion model, Gaussian model, convective boundary layer.

1. INTRODUCTION

Our preoccupation about air pollution is a consequence of the explicit evidence that air contaminants negatively affect the health and the welfare of human beings. Air contaminants concentration influences the health of humans and animals; damage vegetation and materials; reduce visibility and solar radiation; and affect weather and climate [1].

The study and the employment of operational short-range atmospheric dispersion models for environmental impact assessment have demonstrated to be of large use in the evaluation of ecosystems perturbation in many distinct scales [2]. Therefore, short-range atmospheric dispersion models, including the physical description of the Planetary Boundary Layer (PBL), are fundamental tools to evaluate the noxious effect of air pollutants on human health and on urban and agricultural environments [3]. Generally, such air quality short-range models can be useful in predicting contaminants concentration magnitudes in atmospheric boundary layer generated by different forcing mechanisms and consequently distinct degrees of complexity.

In operational applications, the classical Gaussian diffusion models are largely employed in assessing the impacts of existing and proposed sources of air contaminants on local

and urban air quality [1]. Simplicity, associated to the Gaussian analytical model, makes this approach particularly suitable for regulatory usage in mathematical modeling of the air pollution. Indeed, such models are quite useful in short-term forecasting. The lateral and vertical dispersion parameters, respectively σ_y and σ_z , represent the key turbulent parameterization in this approach, once they contain the physical ingredients that describe the dispersion process and, consequently, express the spatial extent of the contaminant plume under the effect of the turbulent motion in the PBL [4].

The following simple algebraic relation has been employed to fit the observed dispersion parameters (σ_y, σ_z) in the PBL under different stability conditions [5-10]:

$$\sigma_\alpha = \frac{\sigma_i t}{\left[1 + \frac{1}{2} \left(\frac{t}{T_{L_i}}\right)\right]^{1/2}} \quad (1)$$

where $\alpha = x, y, z$; $i = u, v, w$, σ_i corresponds to the Eulerian standard deviation of the turbulent wind field, T_{L_i} is the Lagrangian decorrelation time scale and t is the travel time of the fluid particle. Formulation (1) consists of an empirical relationship that satisfies the short and long time limits of Taylor statistical diffusion theory. Its derivation was obtained directly from the fitting of experimental data [11].

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Recently, Degrazia *et al.* [12] showed that the velocity autocorrelation function derived from the functional form (1) satisfies the principal mathematical requirements suggested by Hinze [13] for homogeneous turbulence. Furthermore, this autocorrelation function also satisfies the inertial subrange conditions suggested by Tennekes [14] and Manomaiphiboon and Russel [15]. Based on Kolmogorov's theory [16], this means it captures the n^{-2} frequency falloff in the inertial subrange.

Most of the turbulence parameterizations employed in advanced dispersion models is based on PBL similarity theories [17-20]. Therefore, the dispersion parameters described in terms of a similarity theory are directly related to the basic physical quantities describing the turbulence state of the PBL.

Throughout classical statistical diffusion theory [21], it is possible to relate turbulent parameters in the PBL to spectral distribution of the turbulent kinetic energy. Following such methodology, Degrazia *et al.* [22-23] developed a model for the turbulent spectra in a convective boundary layer and proposed a formulation for the Lagrangian decorrelation time scales and turbulent velocity variances described in terms of the unstable PBL similarity theory.

The following study aims at using Lagrangian decorrelation time scales and turbulent velocity variances, described in terms of the characteristics of the turbulent field in a convective boundary layer, to obtain simple algebraic expressions for the dispersion parameters. The hypothesis to be tested in the present analysis is that complex integral formulations for dispersion parameters, which are only numerically solvable, can be represented by simple algebraic relations constructed from equation (1). To demonstrate that this hypothesis is valid, we compare the values of the lateral and vertical dispersion parameters evaluated from the algebraic expression (1) with those numerically obtained from an integral formulation. Furthermore, the algebraic and integral dispersion parameters are put together with measured values of σ_y and σ_z . As an additional purpose, this paper presents the formulation of a simple short-range Gaussian model which evaluates ground-level concentrations from elevated sources in a boundary layer, dominated by moderate convection. The performance of this Gaussian model incorporating simple algebraic relationships and integral formulations for the lateral and vertical dispersion parameters are compared to ground-level concentrations from atmospheric dispersion experiments that were carried out in the Copenhagen area under moderately unstable conditions [24].

2. ALGEBRAIC AND INTEGRAL FORMULATION FOR THE DISPERSION PARAMETERS

The equation for dimensional Eulerian velocity spectra under unstable conditions in the PBL can be described as a function of convective scales as follows [19],

$$\frac{nS_i^E(n)}{w_*^2} = \frac{1.06c_i f \psi^{2/3} \left(\frac{z}{z_i}\right)^{2/3}}{\left(f_m^*\right)_i^{5/3} \left[1 + 1.5 \left(\frac{f}{\left(f_m^*\right)_i}\right)\right]^{5/3}} \tag{2}$$

where $c_i = \alpha_i (0.5 \pm 0.05) (2\pi k)^{-2/3}$ and $\alpha_i = 1, 4/3, 4/3$ for u, v and w components respectively [25], $k = 0.4$ is von Kármán constant, $f = \frac{nz}{U(z)}$ is the nondimensional frequency, z is the height above the ground, $U(z) = U$ is the horizontal mean wind speed at height z_n , $\left(f_m^*\right)_i$ is the reduced frequency of the convective spectral peak, z_i is the height of the base of the inversion layer capping the daytime convective boundary layer, w_* is the convective velocity scale and the nondimensional molecular dissipation rate function is defined as $\psi = \frac{\epsilon z_i}{w_*^3}$, where ϵ is the mean dissipation rate of turbulent kinetic energy per unit time per unit mass of fluid, with the order of magnitude of ϵ determined only by scales that characterize the energy-containing eddies. Field observations in a convective PBL show that $\psi \approx 0.65$ [26].

The analytical integration of Eq. (2) over the whole frequency domain leads to the following turbulent velocity variance

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$$\sigma_i^2 = \frac{1.06c_i \psi^{2/3} \left(\frac{z}{z_i}\right)^{2/3}}{\left(f_m^*\right)_i^{2/3}} w_*^2 \tag{3}$$

that is employed to normalize the spectrum so that the normalized spectrum can be written as follows:

$$F_i^E(n) = \frac{S_i^E(n)}{\sigma_i^2} = \frac{z}{U\left(f_m^*\right)_i} \left[1 + \frac{1.5f}{\left(f_m^*\right)_i}\right]^{-5/3} \tag{4}$$

Based on a model for the spectra of turbulent kinetic energy and Taylor statistical diffusion theory Degrazia *et al.* [23] derived a mathematical expression for the Lagrangian decorrelation time scale. For non-homogeneous turbulence this decorrelation time scale can be expressed as

$$T_{L_i} = \frac{\beta_i F_i^E(0)}{4} \tag{5}$$

where $\beta_i = \gamma \frac{U}{\sigma_i}$ [27-29] is defined as the ratio of the Lagrangian to the Eulerian decorrelation time scale and $F_i^E(0)$ represents the spectra in which the high frequencies were filtered.

The substitution of the Eq. (3) and Eq. (4) into Eq. (5) and using $\beta_i = \gamma \frac{U}{\sigma_i}$ yields the following expression

$$T_{L_i} = \frac{\gamma}{4} \frac{1}{\sigma_i} \frac{z}{(f_m^*)_i} \tag{6}$$

Finally, the substitution of Eq. (3) and Eq. (6) into Eq. (1) leads to the following generalized algebraic expression for the dispersion parameters

$$\frac{\sigma_\alpha^2}{z_i^2} = \frac{1.06c_i \psi^{2/3} (z/z_i)^{2/3} (f_m^*)_i^{-2/3} X^2}{1 + \frac{2\sqrt{1.06c_i}}{\gamma} \left[\psi^{1/3} (z/z_i)^{-2/3} (f_m^*)_i^{2/3} X \right]} \tag{7}$$

where $X = \frac{xw_*}{Uz_i}$ is a nondimensional distance defined by the ratio of travel time (x/U) to the convective time scale (z_i/w_*). For lateral (σ_y) and vertical (σ_z) dispersion parameters $c_w = c_v = 0.4$. These c_i values derive of the isotropy condition in the inertial subrange. Furthermore, Wandel and Kofoed-Hansen [27] have rigorously shown that for the case of a fully developed isotropic homogeneous turbulence $\gamma = \frac{\sqrt{\pi}}{4}$.

Thusly, the vertical dispersion parameter from elevated sources in an unstable PBL that is first considered. By elevated, we mean that at this height the turbulence structure can be idealized as vertically homogeneous with the length scale of the energy-containing eddies being proportional to the convective boundary layer height z_i , so that the peak vertical wavelength can be written as $(\lambda_m)_w = z_i$ in order to obtain

$$(f_m^*)_w = \frac{z}{(\lambda_m)_w} = \frac{z}{z_i} \tag{8}$$

Therefore, the vertical dispersion parameter for convective conditions can be obtained from Eqs. (7) and (8), employing $c_w = 0.4$ and $\gamma = \frac{\sqrt{\pi}}{4}$, it is expressed as

$$\frac{\sigma_z^2}{z_i^2} = \frac{0.42\psi^{2/3} X^2}{1 + (2.94\psi^{1/3} X)} \tag{9}$$

Experimental observation in a convective boundary layer exhibiting horizontal homogeneity shows that the peak lateral wavelength can be represented by $(\lambda_m)_v = 1.5z_i$ [17]. From this observational consideration yields

$$(f_m^*)_v = \frac{z}{(\lambda_m)_v} = \frac{z}{1.5z_i} \tag{10}$$

Thus, the lateral dispersion parameter for unstable conditions can be constructed from Eqs. (7) and (10) using $c_v = 0.4$ and $\gamma = \frac{\sqrt{\pi}}{4}$ as follows

$$\frac{\sigma_y^2}{z_i^2} = \frac{0.55\psi^{2/3} X^2}{1 + (2.24\psi^{1/3} X)} \tag{11}$$

3. COMPARISON OF THE PROPOSED PARAMETERIZATION WITH A CLASSICAL INTEGRAL FORMULATION DESCRIBING σ_y AND σ_z

To demonstrate that the model as given by (7) is valid, we compare the vertical and lateral dispersion parameters provided respectively by (9) and (11), with the following classical integral formulation proposed by Pasquill and Smith [30] expressing a Lagrangian σ_α in terms of the ratio of the Eulerian energy spectrum to the Eulerian velocity variance as the kernel of a Fourier transform in frequency space:

$$\sigma_\alpha^2 = \frac{\sigma_i^2 \beta_i^2}{\pi^2} \int_0^\infty F_i^E(n) \frac{\sin^2\left(\frac{n\pi t}{\beta_i}\right)}{n^2} dn \tag{12}$$

Substituting Eqs. (3) and (4) and using $\beta_i = \gamma \frac{U}{\sigma_i}$ into Eq. (12), follows that

$$\sigma_\alpha^2 = \frac{1.5\gamma^2}{\pi^2 (f_m^*)_i^2} \left(\frac{z}{z_i}\right)^2 \int_0^\infty \sin^2 \left[\frac{\sqrt{1.06c_i} \pi \psi^{1/3} (f_m^*)_i^{2/3}}{1.5\gamma (z/z_i)^{2/3}} X n' \right] \frac{dn'}{n'^2 (1+n')^{5/3}} \tag{13}$$

where $X = \frac{xw_*}{Uz_i}$ and $n' = \frac{1.5z}{U(f_m^*)_i} n$.

Thus, the vertical dispersion parameter for convective condition can be derived from Eqs. (13) and (8), employing $c_w = 0.4$ and $\gamma = \frac{\sqrt{\pi}}{4}$. This integral formulation for σ_z can be written as

$$\frac{\sigma_z^2}{z_i^2} = \frac{0.29}{\pi^2} \int_0^\infty \frac{\sin^2(0.98\pi\psi^{1/3}Xn')}{n'^2(1+n')^{5/3}} dn' \quad (14)$$

Furthermore, the integral formulation for the lateral dispersion parameter using $c_v = 0.4$, $\gamma = \frac{\sqrt{\pi}}{4}$ and Eq. (10) into Eq. (13), yields

$$\frac{\sigma_y^2}{z_i^2} = \frac{0.66}{\pi^2} \int_0^\infty \frac{\sin^2(0.75\pi\psi^{1/3}Xn')}{n'^2(1+n')^{5/3}} dn' \quad (15)$$

Despite the difference between Eqs. (14) and (15), originated from the turbulence energy spectrum, and Eqs. (9) and (11), which constitute experimental fittings, Figs. (1) and (2) show the existence of a good degree of agreement between the algebraic and integral formulation. Furthermore, in Figs. (1) and (2) the expressions (9), (14), (11) and (15) are compared to the dispersion parameters (σ_z and σ_y) measured in the Copenhagen experiments. In the Copenhagen experiments the contaminants were released without buoyancy from a tower at a height of 115 m and collected at the ground-level positions at a maximum of three crosswind arcs of tracer sampling units. The sampling units were positioned 2 - 6 km from the point of release [24]. The meteorological conditions during the dispersion experiments, ranged from moderately unstable to convective, -43.04 (convective) $< \frac{z_i}{L} < -1.42$ (moderately unstable) [31].

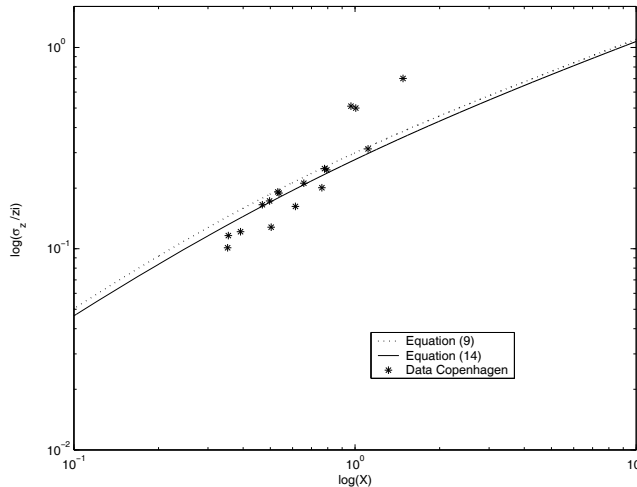


Fig. (1). Vertical dispersion parameter calculated from equations (9) and (14). Asterisks represent values of σ_z/z_i measured in the Copenhagen experiments.

Additionally, using statistical indices Tables 1 and 2 exhibit a comparison of the dispersion parameters (σ_z, σ_y) measured in Copenhagen experiments [24, 31] with those calculated by the equations (9), (11), (14) and (15). From this statistical comparison it can be seen that the simple algebraic formulations reproduce fairly well the observed values of the

lateral and vertical dispersion parameters. An explanation for the distinct statistical indices is given in the appendix.

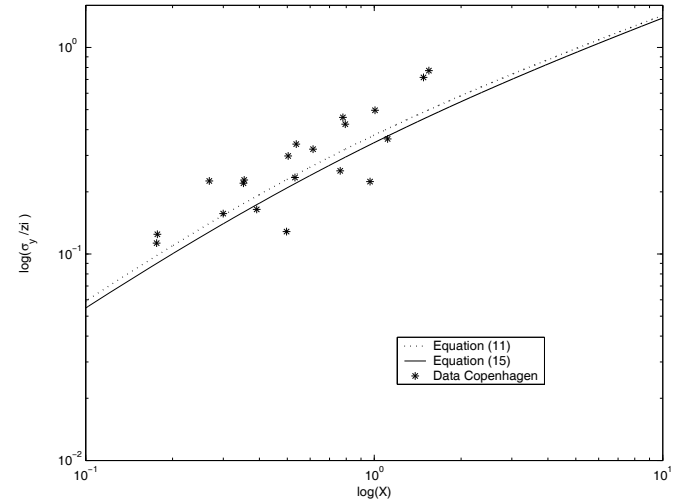


Fig. (2). Lateral dispersion parameter calculated from equations (11) and (15). Asterisks represent values of σ_y/z_i measured in the Copenhagen experiments.

Table 1. Statistical Indices Evaluating the Formulations for σ_z as Given by Equations (9) and (14).

σ_z	NMSE	FB	FS	R	FA2
Equation (9)	0.19	0.05	0.60	0.78	1.00
Equation (14)	0.23	0.14	0.67	0.79	1.00

Table 2. Statistical Indices Evaluating the Formulations for σ_y as Given by Equations (11) and (15)

σ_y	NMSE	FB	FS	R	FA2
Equation (11)	0.12	0.10	0.06	0.73	1.00
Equation (15)	0.14	0.19	0.15	0.73	1.00

Therefore, the present investigation indicates that the dispersion parameters given by simple algebraic interpolation formulas can represent the turbulent dispersion of contaminants released from elevated sources in an unstable boundary layer. The great advantage of using the algebraic expressions for σ_z and σ_y is the fact that these formulas, under the computational point of view, are forty times faster than the numerical integrations and, consequently, they will be useful in the solution of large and complex atmospheric diffusion models.

4. COMPARISON WITH EXPERIMENTAL CONCENTRATION DATA

We evaluate the performance of the algebraic and integral parameterization for σ_z and σ_y dispersion parameters,

applying the Gaussian plume model to the Copenhagen experimental concentration data set. For this comparison were used the measured values of the ground-level crosswind-integrated and the centerline ground-level concentration normalized with the source emission rate [24].

The Gaussian expression for the ground-level crosswind-integrated concentration and the normalized ground-level concentration along the plume centerline are respectively given by [1]

$$\frac{C_y(x,0)}{Q} = \left(\frac{2}{\pi}\right)^{1/2} \frac{1}{U\sigma_z} \exp\left(-\frac{h^2}{2\sigma_z^2}\right) \quad (16)$$

$$\frac{C(x,0,0)}{Q} = \frac{1}{\pi U\sigma_y\sigma_z} \exp\left(-\frac{h^2}{2\sigma_z^2}\right) \quad (17)$$

where Q is the source strength or emission rate and h is the effective height of release above the ground.

The physical fundamental quantities, by the employment of Eq. (16) and Eq. (17), are the vertical and lateral dispersion parameters that are obtained from Eqs. (9), (11), (14) and (15). The substitution of these expressions in Eqs. (16) and (17) provides directly the values of the ground-level concentrations of contaminants released from elevated continuous point sources located in a moderately unstable to convective PBL. Therefore, as a validation of the algebraic formulas for the vertical and crosswind spread of the plume developed in this study, the parameterizations given by the Eqs. (9), (11), (14) and (15) are going to be incorporated in the Gaussian plume model approach defined by Eqs. (16) and (17).

In Tables 3 and 4 the observed ground-level concentrations are exhibited together with computed one from the Gaussian model employing the formulations given by (9), (11), (14) and (15).

Furthermore, Figs. (3) and (4) show respectively the observed and predicted scatter diagram of ground-level crosswind integrated and centerline concentrations using the Gaussian model with vertical and lateral dispersion parameters given by equations (9) and (11) (algebraic formulations) and (14) and (15) (integral formulation).

Finally, the datasets were applied subsequently to the statistical indices ([32], see appendix). Therefore, observing the Figs. (3) and (4) and the statistical indices, Tables 5 and 6, one can easily conclude that the Gaussian model (Eqs. 16 and 17) incorporating the algebraic (Eqs. 9 and 11) and integral formulations (Eqs. 14 and 15) predicts quite well the Copenhagen ground-level observed concentrations. The overall good agreement between Gaussian model predictions using the algebraic formula for the dispersion parameters and field data of ground-level concentration, as well as the comparison with the integral formulation for the σ_z and σ_y , confirms that the simple algebraic relations (9) and (11) contain a realistic description of the energy-containing

eddies that control the turbulent dispersion in the unstable PBL.

Table 3. Observed and Modeled Ground-Level Crosswind Integrated Concentration $C_y(x,0)/Q$ at Different Distances from the Source

Run.	Distance (m)	Data (10^{-4} sm^{-2})	Eqs. (9), (16) (10^{-4} sm^{-2})	Eqs. (14), (16) (10^{-4} sm^{-2})
1	1900	6.48	6.06	6.58
1	3700	2.31	3.96	4.28
2	2100	5.38	3.64	3.79
2	4200	2.95	2.48	2.68
3	1900	8.20	7.35	7.72
3	3700	6.22	5.22	5.60
3	5400	4.30	4.22	4.52
4	4000	11.66	8.54	8.77
5	2100	6.71	6.04	5.71
5	4200	5.84	5.73	5.96
5	6100	4.97	4.90	5.19
6	2000	3.96	3.14	3.18
6	4200	2.22	2.31	2.47
6	5900	1.83	1.90	2.04
7	2000	6.7	3.96	4.25
7	4100	3.25	2.52	2.73
7	5300	2.23	2.14	2.31
8	1900	4.16	4.12	4.28
8	3600	2.02	3.12	3.31
8	5300	1.52	2.56	2.71
9	2100	4.58	3.53	3.70
9	4200	3.11	2.34	2.54
9	6000	2.59	1.85	2.01

5. CONCLUSIONS

Algebraic simple formulations for the lateral and vertical dispersion parameters in an unstable PBL are derived. The development is based upon an empirical algebraic relation in which the turbulent velocity variances and the Lagrangian decorrelation time scales are obtained from the turbulent kinetic energy spectra. By considering the turbulent field structure of the convective boundary layer as fairly homogeneous, that is, the length scale of energy containing eddies proportional to the convective PBL height and the dimensionless turbulent kinetic energy dissipation rate as constant, the present model, describing the dispersion parameters, has been compared with experimental data and with values provided by classical integral formulations which are only numerically solvable.

Table 4. Observed and Modeled Ground-Level Centerline Concentration $C(x, 0, 0) / Q$ at Different Distances from the Source

Run.	Distance (m)	Data (10^{-7} sm^{-3})	Eqs. (9), (11), (17) (10^{-7} sm^{-3})	Eqs. (14), (15), (17) (10^{-7} sm^{-3})
1	1900	10.50	5.34	6.37
1	3700	2.14	2.17	2.55
2	2100	9.85	7.67	8.71
2	4200	2.83	2.93	3.48
3	1900	16.33	13.74	15.87
3	3700	7.95	5.95	6.98
3	5400	3.76	3.72	4.32
4	4000	15.71	17.51	19.36
5	2100	12.11	20.94	21.73
5	4200	7.24	11.49	13.14
5	6100	4.75	7.52	8.69
6	2000	7.44	8.02	8.91
6	4200	3.37	3.24	3.80
6	5900	1.74	2.07	2.44
7	2000	9.48	5.55	6.54
7	4100	2.62	2.03	2.41
7	5300	1.15	1.44	1.70
8	1900	9.76	8.43	9.62
8	3600	2.64	4.06	4.69
8	5300	0.98	2.59	2.96
9	2100	8.52	6.86	7.85
9	4200	2.66	2.55	3.04
9	6000	1.98	1.53	1.83

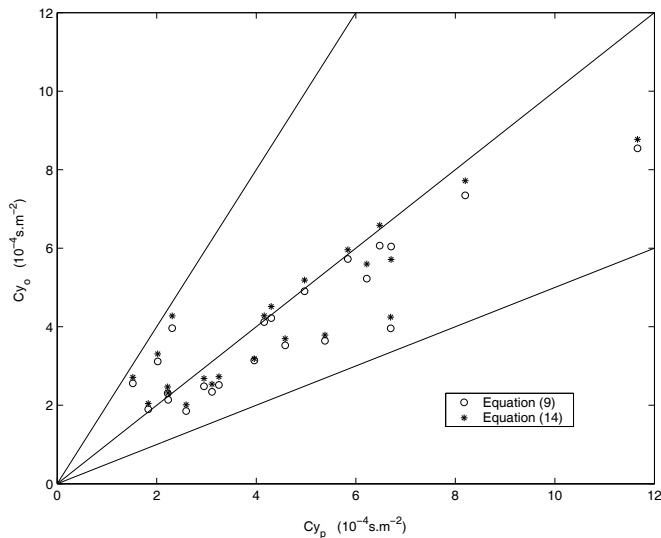


Fig. (3). Observed (C_{y_o}) and predicted (C_{y_p}) ground-level crosswind integrated concentration, normalized with emission rate $C_y(x, 0) / Q$: scatter diagram for the solution of Eq. (16) using Eqs. (9) and (14).

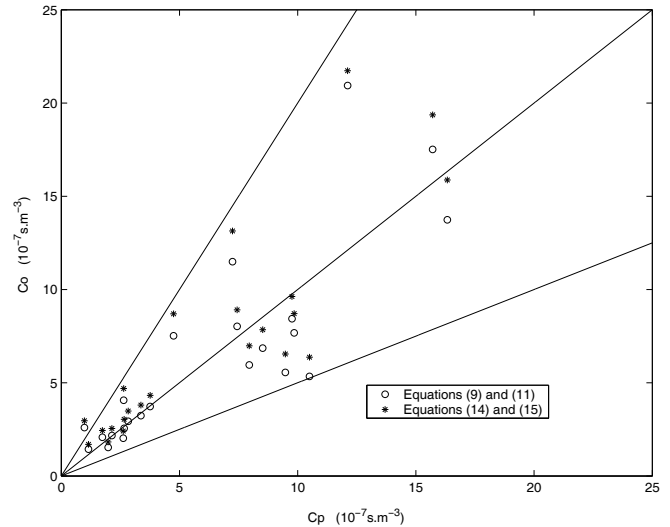


Fig. (4). Observed (C_o) and predicted (C_p) ground-level centerline concentration, normalized with emission rate $C(x, 0, 0) / Q$: scatter diagram for the solution of Eq. (17) using Eqs. (9), (11), (14) and (15).

Table 5. Statistical Indices Evaluating the Model Performance Given by Equations (16), (9) and (14)

$C(x, 0) / Q$	NMSE	FB	FS	R	FA2
Equation (9)	0.08	0.12	0.30	0.91	1.00
Equation (14)	0.06	0.07	0.28	0.91	1.00

Table 6. Statistical Indices Evaluating the Model Performance Given by Equations (17), (9), (11), (14) and (15)

$C(x, 0, 0) / Q$	NMSE	FB	FS	R	FA2
Equations (9) and (11)	0.19	-0.01	-0.12	0.84	0.96
Equations (14) and (15)	0.19	-0.14	-0.19	0.86	0.96

This comparison shows that the lateral and vertical dispersion parameters calculated from the simple algebraic formulas (Eqs. (9) and (11)) can describe the turbulent diffusion process in an unstable PBL.

Furthermore, by using a Gaussian plume model and a dataset of diffusion experiments performed in an unstable PBL, ground-level contaminant concentrations calculated using the dispersion parameters given by the algebraic simple formulations (Eqs. (9) and (11)) were compared to the ones obtained by the classical integral formulation derived by Pasquill and Smith [30] (Eqs. (14) and (15)).

The validations used in this study show that the Gaussian short range dispersion model employing the algebraic formulas for the lateral and vertical dispersion parameters reproduces well the measured concentrations from contaminants released from elevated continuous point sources situated in a moderately unstable to convective boundary layer. Therefore, the simple algebraic formulation for dispersion parame-

ters can be used as a surrogate parameterization for the complex integral formulation.

As a consequence of the analyticity of the expression (1) its use in dispersion models removes problems associated to the computational time and mathematical approximation. Therefore, the new algebraic dispersion parameters may be suitable for applications in regulatory air pollution short range dispersion model.

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Appendix

Following Hanna [32] the statistical indices used in this study are defined as:

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

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

$$FS = 2(\sigma_o - \sigma_p) / (\sigma_o + \sigma_p) \text{ (Standard Fractional Bias)}$$

$$R = \frac{(\overline{C_o} - \overline{C_o})(\overline{C_p} - \overline{C_p})}{\sigma_o \sigma_p} \text{ (Correlation Coefficient)}$$

$$FA2 = 0.5 \leq C_o / C_p \leq 2 \text{ (Factor of 2)}$$

where C is the analyzed amount and the subscript "o" and "p" refer to observed and predicted quantities, respectively, the over bar indicates an averaged value. The statistical index FB says if the predicted quantity underestimates or overestimates the observed ones. The statistical index $NMSE$ represents the quadratic error of the predicted quantities related to the observed ones. The statistical index FS indicates the as the model gets to simulate the dispersion of the observed data. The statistical index $FA2$ supply the fraction of the data for the ones which $0.5 \leq C_o / C_p \leq 2$. The best results are expected to have values near zero for the indices $NMSE$, FB and FS and near 1 in the indices R and $FA2$.