Modelling dispersion from elevated sources in a planetary boundary layer dominated by moderate convection

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Summary. — A general method to evaluate dispersion parameters for a turbulent Planetary Boundary Layer (PBL) under convective conditions is described in this paper. The method is based on Taylor's diffusion theory. By employing the Gaussian plume approach the model performances are evaluated against experimental ground-level concentrations.

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1. – Introduction

The Gaussian plume model concept is still important for estimating ground-level concentrations due to tall stack emissions and is usually suitable for regulatory use in air quality models [1]. Recently, much effort has been put into the development of non-Gaussian models, such as Lagrangian particle models (*e.g.*, Anfossi *et al.* [2], De Baas *et al.* [3], Weil [4]) and large-eddy models [5, 6]. These models can describe non-homogeneous atmospheric structures and also handle tracer dispersion in complex flow, but they result in excessively long computer runs for calculating concentration time series over a long time (*e.g.*, a year), which is important in the evaluation of the violations of air pollution standards.

Improved dispersion algorithms in updated Gaussian models calculate the dispersion parameters σ_y and σ_z in terms of distinct scaling parameters for turbulence. These scaling parameters such as friction velocity (u_*), Monin-Obukhov length scale (L), convective velocity scale (w_*) and convective boundary-layer height (z_i) are frequently used in expressions to calculate the lateral (σ_y) and the vertical (σ_z) dispersion parameters. Models that are based on these parameters are the OML model [7], the PPSP model [8] and the HPDM model [9].

According to Weil [10], "For elevated releases in a boundary layer with moderate convection, dispersion modeling is on a more tentative basis because of our incomplete knowledge of the turbulence structure, and limited model testing. For the present, the Gaussian plume model may be sufficient."

In this context the present study shows a practical short-range Gaussian model evaluating ground-level concentrations from elevated sources in a boundary layer dominated by a moderate convection. Taylor's statistical diffusion and the convective similarity theories are used to derive a general expression for the dispersion parameters. It is known that Taylor's theory performs well on experimental data, when the measurements of turbulent diffusion from the individual experiments are used. For instance, the interpolations formulas from Venkatram *et al.* [11] and Briggs [12] represent empirical fitting curves obtained from a collection of dispersion parameters measured in the planetary boundary layer. The aim in this study is to use Taylor's theory to construct a relation for the dispersion parameters that is described only in terms of the characteristics of the turbulent field in a Convective Boundary Layer (CBL). Therefore, the Gaussian plume model incorporates improved formulations of the dispersion parameters σ_y and σ_z. It is assumed here that the spectral forms for the turbulent velocities presented by Degrazia *et al.* [13] give a good description of the energy distribution in a CBL. The model performances are evaluated against ground-level concentrations using atmospheric dispersion experiments that were carried out in the northern part of Copenhagen under moderate unstable conditions [14].

2. – Model development

The dispersion parameters are statistical quantities of much interest in dispersion modeling. They are defined in terms of the second moments of particle displacements in the x, y and z directions [15]. Our formulation starts with the equation for the generalized dispersion parameter $\overline{\mathbf{X}^2}$ as given by Pasquill and Smith [16],

$$\overline{\mathbf{X}^2} = \frac{\sigma_i^2 \beta_i^2}{\pi^2} \int_0^\infty S_i(n) \frac{\sin^2(\pi n t/\beta_i)}{n^2} \, \mathrm{d}n , \tag{1}$$

where $\mathbf{X}$ corresponds to the position vector for each particle, the overbar indicates an ensemble average over a large number of particles, σ_i corresponds to the Eulerian standard deviation of the i component of turbulent wind field (i can be substituted by u, v or w), β_i is defined as the ratio of the Lagrangian to the Eulerian integral time scales, $S_i(n)$ is the value of the spectrum of energy normalized by the Eulerian variance velocity, t is the travel time and n is the frequency.

According to Wandel and Kofoed-Hansen [17],

$$\beta_i = \left(\frac{\pi U^2}{16\sigma_i^2} \right)^{1/2} \tag{2}$$

is a function of the mean wind speed U and the turbulence intensity (variance) and varies from 10 for stable conditions to 2 for convective conditions [18].

The Eulerian velocity spectra under unstable conditions can be expressed as a function of convective scales [13, 19], as follows:

$$\frac{nS_i(n)}{w^2_*} = \frac{0.98c}{(f_m)_i^{5/3}}\frac{f}{q}\left[1+\frac{1.5}{(f_m)_i}\frac{f}{q}\right]^{-5/3}\left(\frac{\psi_\varepsilon}{q}\right)^{2/3}\left(\frac{z}{z_i}\right)^{2/3}, \tag{3}$$

where c is equal to $\alpha_1(2\pi\kappa)^{-2/3}$ κ is the von Karman constant, α_1 is evaluated experimentally from the spectrum for each wind component so that c assumes the values 0.3 for the u component and 0.4 for the v and w components, f is the reduced frequency (nz/U), z is the height above the surface, $(f_m)_i$ is the frequency of the spectral peak in the neutral stratification, $q=(f_m^*)_i(f_m)_i^{-1}$ is a stability function where $(f_m^*)_i$ is the frequency of the spectral peak regardless of the stratification, z_i is the convective PBL height, (w_*) is the convective velocity scale and $\psi_\varepsilon = \varepsilon z_i/{w_*}^3$ is the nondimensional molecular dissipation rate function. ε is the ensemble-average rate of dissipation of turbulent kinetic energy.

By analytically integrating eq. (3) over the whole frequency domain, one can obtain the variance that is used to normalize the spectrum

$$\sigma_i^2 = \frac{0.98c}{(f_m)_i^{2/3}}\left(\frac{\psi_\varepsilon}{q}\right)^{2/3}\left(\frac{z}{z_i}\right)^{2/3}w_*^3, \tag{4}$$

so that the value of the normalized Eulerian spectrum can be given by

$$S_i(n) = \frac{1}{(f_m)_i}\frac{z}{Uq}\left[1+\frac{1.5}{(f_m)_i}\frac{nz}{Uq}\right]^{-5/3}. \tag{5}$$

A general formulation for the dispersion parameters can now finally be obtained from eqs. (1), (2), (4) and (5) and be expressed as

$$\frac{\overline{\mathbf{X}^2}}{z_i^2} = \frac{1.5(z/z_i)^2}{16\pi(f_m)_i^2q^2}\int_0^\infty \frac{\sin^2\left[\dfrac{4\sqrt{\pi}(0.98c)^{1/2}\{(f_m)_i^2q^2\psi_\varepsilon\}^{1/3}Xn'}{1.5(z/z_i)^{2/3}}\right]}{n'^2(1+n')^{5/3}}\,\mathrm{d}n', \tag{6}$$

where $X \equiv w_* x/Uz_i$ can be thought of as a nondimensional time since it is the ratio of travel time (x/U) to the convective time scale (z_i/w_*). x is the dimensional distance downwind.

Thusly, the vertical dispersion parameter from elevated sources in an unstable PBL 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

$$q = \frac{(f_m^*)_w}{(f_m)_w} = \frac{z}{(\lambda_m)_w 0.35} = 2.86\frac{z}{z_i}, \tag{7}$$

where $(f_m)_w$ is equal to 0.35 [19]. To proceed, the vertical dispersion parameter for convective conditions can be obtained from eqs. (6) and (7), using $c=0.4$ and $(f_m)_w = 0.35$

and be expressed as

$$\frac{\sigma_z^2}{z_i^2} = \frac{0.093}{\pi} \int_0^\infty \frac{\sin^2(2.96\,\psi_\varepsilon^{1/3} X n')}{(1+n')^{5/3} n'^2}\, \mathrm{d}n' \, . \tag{8}$$

For completeness, the lateral dispersion parameter for convective conditions is now specified. Therefore, using the peak lateral wavelength $(\lambda_m)_v = 1.5 z_i$ [20, 21], $c = 0.4$ and $(f_m)_v = 0.16$ [19], the lateral dispersion parameter can be obtained from eq. (6) with

$$q = \frac{(f_m^*)_v}{(f_m)_v} = \frac{z}{(\lambda_m)_v 0.16} = 4.16\, \frac{z}{z_i} \tag{9}$$

and be expressed as

$$\frac{\sigma_y^2}{z_i^2} = \frac{0.21}{\pi} \int_0^\infty \frac{\sin^2(2.26\,\psi_\varepsilon^{1/3} X n')}{(1+n')^{5/3} n'^2}\, \mathrm{d}n' \, . \tag{10}$$

3. – Evaluation against results of the Gaussian model and experimental data

The model performance has been evaluated against experimental ground-level concentrations using tracer SF_6 data from dispersion experiments carried out in the northern part of Copenhagen, described in Gryning *et al.* [22]. The tracer was released without buoyancy from a tower at a height of 115 m, and collected at the ground-level positions in up to three crosswind arcs of tracer sampling units. The sampling units were positioned 2–6 km from the point of release. Tracer releases typically started 1 h before the start of tracer sampling and stopped at the end of the sampling period; the average sampling time was 1 h. The site was mainly residential with a roughness length of 0.6 m. Table I shows the data (from Gryning and Lyck [14] and Gryning *et al.* [22]) utilized for the validation of the proposed model. The meteorological data used were collected near the ground, so the comparison can be said to simulate the values given

TABLE I. – *Meteorological data.*

Exp no.	U (ms^{-1})	u_* (ms^{-1})	L (m)	w_* (ms^{-1})	z_i (m)	z^s/z_i	z_i/L
1	3.40	0.37	−46	1.76	1980	0.058	−43.00
2	10.60	0.74	−384	1.72	1920	0.060	−5.00
3	5.00	0.39	−108	1.15	1120	0.103	−10.00
4	4.60	0.39	−173	0.69	390	0.295	−2.30
5	6.70	0.46	−577	0.70	820	0.140	−1.42
6	13.20	1.07	−569	1.91	1300	0.088	−2.30
7	7.60	0.65	−136	2.11	1850	0.062	−14.00
8	9.40	0.70	−72	2.13	810	0.142	−11.00
9	10.50	0.77	−382	1.84	2090	0.055	−5.50

by a routine use of the model. The stability parameter z_i/L indicates cases of moderate convection. To calculate w_*, in table I, the relation $w_*/u_* = (-z_i/\kappa L)^{1/3}$ was used.

As in table I the stability parameters z_i/L and U/w_* indicate cases of moderate to slight convection (stability categories B and C), it seems appropriate to incorporate eqs. (8) and (10) in the Gaussian model to simulate the ground-level concentrations [10].

The hypothesis assumed in this work is that for elevated releases in moderate convection the vertical concentration distribution can be approximated by a Gaussian.

The Gaussian expression for the crosswind-integrated concentration can be written as [23]

$$c_y(x, z) = \frac{Q}{\sqrt{2\pi}\,\sigma_z U}\left[\exp\left[-\frac{(z - z^s)^2}{2\sigma_z^2}\right] + \exp\left[-\frac{(z + z^s)^2}{2\sigma_z^2}\right]\right], \tag{11}$$

where Q is the continuous point source strength, z^s is the effective emission height and σ_z is the vertical spread of the plume. Therefore, when the crosswind-integrated concentration at the surface $c_y(x, 0)$ is known, the concentration at the surface can be confidently calculated at any point using the standard Gaussian model for lateral concentrations

$$c(x, y, 0) = \frac{c_y(x, 0)}{\sqrt{2\pi}\,\sigma_y}\exp\left[-y^2/2\sigma_y^2\right], \tag{12}$$

where y is the crosswind distance and σ_y is the crosswind spread of the plume.

The basic functions, by the employment of (11) and (12), are the vertical and lateral dispersion parameters that can be obtained from eqs. (8) and (10).

Both eqs. (8) and (10) contain the unknown function ψ_ε. This molecular dissipation of turbulent velocity is one of the leading destruction terms in equations for the budget of second-order moments. Therefore, the PBL evolution is dependent on this function. Observations and numerical simulations in central regions of the CBL show that $\psi_\varepsilon \cong 0.4$ [21, 24, 25]. Nevertheless, several field experiments in a CBL [20, 21, 26-28] emphasize that for dimensionless heights in the range $0.05 < z/z_i < 0.3$ the values of ψ_ε are much greater than 0.4.

Following Druilhet *et al.* [27], the profile of the ψ_ε can be approximated by the exponential law:

$$\psi_\varepsilon = 1.26\exp\left[-\frac{z}{0.8z_i}\right], \qquad 0 < z/z_i < 0.8\,. \tag{13}$$

On the other hand, based on the Minnesota and Aschurch experiments [21], the dissipation function ψ_ε can be described as follows [29]:

$$\psi_\varepsilon = 1.5 - 1.2(z/z_i)^{1/3}\,. \tag{14}$$

TABLE II. – *Observed and estimated ground-level crosswind-integrated concentrations* $c_y(x, 0)/Q$ *at different distances from the source. The model uses eqs.* (8) *and* (11).

Exp no.	Distance (km)	Data (10^{-4} s m^{-2})	Model (10^{-4} s m^{-2})
1	1.9	6.48	6.32
	3.7	2.31	4.10
2	2.1	5.38	3.71
	4.2	2.95	2.58
3	1.9	8.20	7.53
	3.7	6.22	5.40
	5.4	4.30	4.35
4	4.0	11.66	8.65
5	2.1	6.71	6.14
	4.2	5.84	5.63
	6.1	4.97	4.78
6	2.0	3.96	3.19
	4.2	2.22	2.39
	5.9	1.83	1.97
7	2.0	6.70	4.10
	4.1	3.25	2.62
	5.3	2.23	2.22
8	1.9	4.16	4.21
	3.6	2.02	3.20
	5.3	1.52	2.62
9	2.1	4.58	3.60
	4.2	3.11	2.44
	6.0	2.59	1.93

Finally, Guillemet *et al.* [28] suggest the following fitting curve for the dissipation rate of turbulent kinetic energy:

$$\psi_\varepsilon = [0.55 + 0.05(z/z_i)^{-2/3}]^{3/2}, \qquad 0.03 < z/z_i < 0.3 . \tag{15}$$

Considering this set of field experiments and the dimensionless source heights (z^s/z_i) used in Copenhagen (table I), it is possible to choose for $\psi_\varepsilon^{1/3}$ in eqs. (8) and (10) an average value. Since the model needs only $\psi_\varepsilon^{1/3}$, this approximation is unlikely to introduce significant errors.

Actually, calculating $\psi_\varepsilon^{1/3}$ from eqs. (13), (14) and (15) in the source heights of the Copenhagen releases, values with no significant differences are obtained, yielding an average value for $\psi_\varepsilon^{1/3}$ equal to 0.97.

As a test for the model, the parameterizations (8) and (10) with $\psi_\varepsilon^{1/3} = 0.97$ are going to be incorporated in the Gaussian plume approach defined by (11) and (12).

In tables II and III the measured ground-level concentrations are presented together with the computed ones of the Gaussian model.

Analysing tables II and III, it can be seen that the Gaussian model results, along with the vertical, eq. (8), and lateral, eq. (10), dispersion parameters, adequately describe the observed ground-level concentrations.

TABLE III. – *Observed and estimated centerline ground-level concentrations* $c(x, 0, 0)/Q$ *at different distances from the source. The model uses eqs.* (10) *and* (12).

Exp no.	Distance (km)	Data (10^{-7} s m^{-3})	Model (10^{-7} s m^{-3})
1	1.9	10.50	5.81
	3.7	2.14	2.33
2	2.1	9.85	8.05
	4.2	2.83	3.17
3	1.9	16.33	14.67
	3.7	7.95	6.41
	5.4	3.76	3.97
4	4.0	15.71	18.27
5	2.1	12.11	13.87
	4.2	7.24	7.60
	6.1	4.75	5.00
6	2.0	7.44	8.42
	4.2	3.37	3.49
	5.9	1.74	2.24
7	2.0	9.48	5.98
	4.1	2.62	2.20
	5.3	1.15	1.55
8	1.9	9.76	9.00
	3.6	2.64	4.32
	5.3	0.98	2.74
9	2.1	8.52	7.20
	4.2	2.66	2.76
	6.0	1.98	1.66

TABLE IV. – *Statistical evaluation of model results.*

Model	NMSE	r	FB	FS
$c_y(x, 0)$	0.08	0.87	0.10	0.31
$c(x, 0, 0)$	0.08	0.88	0.06	0.07

Moreover, table IV presents some statistical indices defined as follows:

$$\text{normalized mean-square error: (NMSE)} = \frac{\overline{(c_\mathrm{m} - c_\mathrm{obs})^2}}{\overline{c_\mathrm{obs}} \cdot \overline{c_\mathrm{m}}} \,,$$

$$\text{correlation coefficient: } (r) = \frac{\overline{(c_\mathrm{m} - \overline{c_\mathrm{m}})(c_\mathrm{obs} - \overline{c_\mathrm{obs}})}}{\sigma_\mathrm{m}\sigma_\mathrm{obs}} \,,$$

$$\text{fractional bias: (FB)} = 2\,\frac{\overline{c_\mathrm{m}} - \overline{c_\mathrm{obs}}}{\overline{c_\mathrm{m}} + \overline{c_\mathrm{obs}}} \,,$$

$$\text{fractional standard deviation: (FS)} = 2\,\frac{\sigma_\mathrm{m} - \sigma_\mathrm{obs}}{\sigma_\mathrm{m} + \sigma_\mathrm{obs}} \,,$$

where c_{obs} and c_{m} are the observed and model concentrations, respectively, while σ is the standard deviation.

As one can easily note, the statistical indices illustrate that the model performs quite well. They confirm also the reliability of the dispersion parameters and, as a consequence, the prominent feature of Taylor's theory, that in the near field (small travel times) $\sigma^2_{y,z} \propto t^2$ and in the far field, $\sigma^2_{y,z} \propto t$.

4. – Conclusions

A general formulation for the dispersion parameters in a CBL is proposed. The method is based upon a model for the spectra of turbulent kinetic energy and Taylor statistical diffusion theory. These multiple-dispersion parameters, one for each different spatial direction, are expressed as functions of the convective similarity coordinates, the nondimensional molecular dissipation rate and the frequency of the spectral peak in the unstable stratification.

By considering the turbulence structure of the CBL as fairly homogeneous, *i.e.* the length scale of the energy containing eddies proportional to the convective PBL height and the dimensionless turbulent kinetic energy dissipation rate as constant, it was possible to describe the dispersion parameters as only universal functions of the nondimensional distance X. A preliminary evaluation of the dispersion parameters performance, based on the Gaussian plume model, using experimental ground-level concentrations and, as input, meteorological data collected near the ground produced good results.

The analysis of the results presented in tables II and III shows that eqs. (8) and (10) may be considered as dispersion parameters to be utilized in applied air quality dispersion models.

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