A new formulation of σ_y and σ_z for air quality dispersion models

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Abstract

A general formulation for estimating dispersion parameters σ_y and σ_z in the Planetary Boundary Layer (PBL) is proposed. These parmeterizations can be utilised in Gaussian air quality dispersion models for regulatory applications.

They are based on the classical Taylor's statistical diffusion theory and on the modelled turbulent kinetic energy spectra and represents an extension of previous models (Degrazia et al.[1,2]) which were mainly focused on dispersion in a purely convective or in a purely mechanic boundary layer. The sigmas proposed here allow to treat the dispersion in a boundary layer where both buoyancy and shear are important forcing mechanisms. The improved parameterization, inserted in a Gaussian model, has been validated using SF_6 tracer data taken from dispersion experiments.

1 Introduction

The Gaussian dispersion plume models are still the most widely used models to estimate ground-level concentrations due to tall stacks emissions. Most regulatory models recommended by EPA, utilised in European countries, are based on the Gaussian assumptions concerning the concentration distribution in both the horizontal and vertical directions. In spite of their simplicity, of their simple input requirements

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they produce results that match experimental data as well as any other model. These models are used in short-term (hourly, daily) as well as long term (seasonal, annual) applications.

Recently, much effort has been put into development of more sophisticated mathematical and models, K-models, Lagrangian particles models, large eddy models which could also handle non-homogeneous atmospheric structures, but notwithstanding the availability and affordability of faster computer, they still result in excessively long computer runs for calculating concentration time series over a long time which is important in the evaluation of the violations of air pollution standards (Bowen[3]).

In order to make use of Gaussian expression, air pollution standard deviations have to be specified. In the past, several methods to model the dispersion parameters σ_y and σ_z have been proposed. They were all based both on theory than in empirical evidence from experimental data.

In this paper we present a method to deduce the dispersion parameters following a model recently proposed by Degrazia et al.[1,2]. Such model was based on classical Taylor's theory in which the turbulent velocity spectra were modelled considering separately the buoyancy and shear generated PBL. The present method is applicable to an intermediate PBL generated by both forcing mechanism, thus it can be applicable to a wider range of PBL stability regimes and for sources of pollutant placed everywhere.

Furthermore the parameterization proposed allows to express the dispersion parameters in terms of the universal characteristics of the turbulent field of the Planetary Boundary Layer eliminating the necessity of dispersion parameters fitting from diffusion experiments.

The dispersion parameters, inserted in a Gaussian model, have been evaluated using the measured concentration data at the sites Copenhagen (Gryning and Lick[4]) and Kincaid (Bowne and Lodergan[5]). Results are then compared with those obtained by the air dispersion models HPDM (Hanna and Chang[6]) and OML (Berkowicz et al.[7]).

2 Dispersion coefficients

The dispersion parameters are defined in terms of the second moments of particle displacements in the x, y and z directions. Our formulation starts with the equation for the generalized dispersion parameter $\overline{\mathbf{X}^2}$ as given by Pasquill and Smith[8].

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

where **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 timescales, $S_i(n)$ 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[9]

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

is a function of the mean wind speed U and of wind variance σ_i and varies from 10 for stable conditions to 2 for convective conditions. Providing the Eulerian turbulent spectra we can solve eqn.1 and calculate the dispersion parameters.

Recently some of the authors have developed a spectral formulation for the turbulent velocities in a purely mechanical driven PBL (Degrazia et al.[2]) and in a convective PBL in terms of fundamental scaling parameters (Degrazia et al.[1]). More details can be found in the above cited papers, whereas in the following a brief description will be given with the extension to a shear-buoyancy driven PBL.

The Eulerian velocity spectra under unstable conditions can be expressed as a function of convective scales (Olesen et al.[10] Degrazia et al.[1]) as follows:

$$\frac{nS_i^E(n)}{w_*^2} = \frac{0.98c}{(f_m)_i^{5/3}} \frac{f}{q_i} \left[1 + \frac{1.5}{(f_m)_i} \frac{f}{q_i} \right]^{-5/3} \left(\frac{\psi_\varepsilon}{q_i} \right)^{2/3} \left(\frac{z}{z_i} \right)^{2/3} \qquad (2)$$

where c is equal to c=0.4 for v and w spectra, 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, ($(f_m)_v = 0.16$ and $(f_m)_w = 0.33$), $q_i = (f_m^*)_i (f_m)_i^{-1}$, is a stability function where $(f_m^*)_i$ is the frequency of the spectral peak regardless of the stratification, in particular we have $q = 4.16 \frac{z}{z_i}$, and $q_w = 1.68 \left(\frac{z}{z_i} \right) \left[1 - \exp\left(-4 \frac{z}{z_i} \right) - 0.0003 \exp\left(\frac{8z}{z_i} \right) \right]^{-1}$, $\psi_\varepsilon = \varepsilon z_i / w_*^3$ is

the non dimensional molecular dissipation rate function, ε is the ensemble- average rate of dissipation of turbulent kinetic energy.
Following local similarity arguments the Eulerian velocity spectra under stable conditions can be written as

$$\frac{nS_i^E(n)}{U_*^2} = \frac{1.5c_i}{(f_m)_i^{5/3}} \frac{f/q_i \left(\Phi_\varepsilon / q_i\right)^{2/3}}{\left[1 + \frac{1.5}{(f_m)_i^{5/3}} \left(\frac{f}{q_i}\right)^{5/3}\right]} \tag{3}$$

where U_* is the local friction velocity, $q_i \equiv \frac{(f_m^*)_i}{(f_m)_i} = \left(1 + 3.7\frac{z}{\Lambda}\right)$ and Λ is the local Obukhov length.
An intermediate PBL is one in which the turbulent eddies are generated by both the above mentioned forcing mechanisms. Making use of the hypothesis of superposition (Hoistrup[11], Berkowicz and Prahm[12]) and neglecting the effects of the interaction shear/buoyancy on the mean field (Moeng and Sullivan[13]) then the turbulent PBL spectra can be expressed as the superposition of a buoyancy and shear produced parts each one scaled with the appropriates velocity scales:

$$S_i^E(n) = S_{ib}^E(n) w_*^2 + S_{is}^E(n) u_*^2$$

where now the buoyant turbulent part is given by

$$\frac{nS_{ib}^E(n)}{w_*^2} = \frac{0.98c_i f}{\left(f_m^*\right)_i^{5/3} \left[1 + 1.5\frac{f}{(f_m^*)_i}\right]^{5/3}} \left(\Psi_{\varepsilon b}\right)^{2/3} \left(\frac{z}{h}\right)^{2/3} \tag{4a}$$

while the mechanical component of spectrum is the same as neutral limit of eqn.3:

$$\frac{nS_{is}^E(n)}{u_*^2} = \frac{1.5c_i f}{(f_m)^{5/3} \left[1 + \frac{1.5 f^{5/3}}{\left(f_m\right)^{5/3}}\right]} \Psi_{\varepsilon s}{}^{2/3} \tag{4b}$$

in which the dissipation rate $\Psi_{\varepsilon s} = \varepsilon_s kz / u_*^3$ is adimensionalized with surface layer scaling parameters.
The total dissipation rate function still can be obtained as sum of two parts each one related to the corresponding turbulence generating mechanism (Hoistrup[11]):

$$\varepsilon = \varepsilon_b + \varepsilon_s = 0.75^{3/2} \frac{w_*^3}{h} + \frac{u_*^3}{kz}\left(1 - \frac{z}{h}\right)^3$$

Eqns. 2, 3, 4a and 4b let us to model the turbulent spectra and, consequently, to express the dispersion parameters in a wide range of atmospheric stability regimes.

3 Evaluation against experimental data

The dispersion parameters, inserted in the well-known Gaussian plume formulation, have been evaluated against ground level concentration data from two different field campaigns, concerning buoyant and non buoyant emission in different atmospheric stability conditions, and different geographical characteristics.
The concentration field is thus given by

$$c(x,y,z) = \frac{c_y(x,z)}{\sqrt{2\pi}\sigma_y} \exp(-y^2 / 2\sigma_y^2) \tag{5}$$

where c_y is the cross-wind integrated concentration

$$c_y(x,z) = \frac{Q}{\sqrt{2\pi}\sigma_z U}\left[\exp\left\{-\frac{(z-h_{eff})^2}{2\sigma_z^2}\right\} + \exp\left\{-\frac{(z+h_{eff})^2}{2\sigma_z^2}\right\}\right] \tag{6}$$

where Q is the source strength, h_{eff} is the effective emission height: $h_{eff} = h_s + \Delta h$, where Δh is the final plume rise. Reflection from the top is assumed.

3.1 Field data

The field data utilised to test the model were selected from two field experiments on atmospheric dispersion according to the protocol agreed at the Manno Workshop (Cuvelier[14]).
1.The Copenhagen data set (Gryning[4]) involved an elevated non buoyant SF_6 release in a mainly residential area. The surface sampling arrays were positioned in arcs from 2 to 6 km downwind of the source.
2. The Kincaid field campaign (Bowne and Londergan[5])concerns an elevated buoyant release in a flat farmland with some lakes. During the experiment, SF_6 was released from a 187 tall stack and recorded on a network consisting of roughly 200 samplers. Only data with a quality factor 3 were considered.
The main characteristics of the two field experiments are listed in Table 1.

3.2 Model evaluation

The model was evaluated by comparing predicted and measured ground level concentration along the plume centreline.
For the buoyant plume cases, the plume rise was calculated following Briggs[15] including the Briggs'1980 criteria for plume penetration of elevated stable layers. (Weil and Brower[16]). The internal turbulence in the plume induced by buoyancy has been estimated according to Briggs[15] as

$$\sigma_{eff} = (\sigma^2 + \Delta h^2 / 2\pi)^{1/2}$$

Table 1: Characteristics of the three sites used for model evaluation.

Site Name	Source	Number of monitors (distance from source)	Surrounding Terrain	Atmospheric conditions
Copenhagen	115 m non-buoyant	About 60 (2-6 km)	flat-mainly residential	From convective to neutral
Kincaid	187 m buoyant	about 200 (0.5-50 km)	Flat farmland, some lakes	From convective to stable

The model performances measures are obtained using the statistical evaluation procedure software described by Hanna[18] and are defined in the following way

cor (correlation)= $\overline{(C_o - \overline{C_o})(C_p - \overline{C_p})} / \sigma_o \sigma_p$

fa2 = fraction of C_o values within a factor two of corresponding C_p values

fb (fractional bias)= $\left(\overline{C_o} - \overline{C_p}\right) / \left(0.5\left(\overline{C_o} + \overline{C_p}\right)\right)$

where subscripts o and p refer to observed and predicted quantities, and an overbar indicates an average.
Measured data are compared with model predictions in figs.1-2, respectively for Copenhagen, Kincaid. The statistical indexes are summarised in Tables 2-3 and compared with the ones obtained by two other next generation models tested on the same experimental data (Olesen[17]). For the Copenhagen dataset, the agreement between predictions and data is very good, also the statistical indexes indicate a better performances of the Gaussian model as proposed and the HPDM (Hanna and Chang[6]) and the OML (Berkowikcz et al. [7]). For the Kincaid dataset the scatter between data and model is bigger than the previous

case, the agreement is less good and the correlation factor is quite low, about 0.36. This can be due 1) to the much stochastic variability existing in the observations and 2) to some simplifications in the description of buoyant plumes. Anyway, the fa2 is 66%, and the model performance are still comparable with the two other models that have a more complex structure than the Gaussian model here considered.

Table 2 Copenhagen data set. Summary of performance measures for maximum arcwise concentrations.

	Nmse	Cor	Fa2	Fb
the presented model	0.10	0.92	96%	0.092
HPDM	0.61	0.87	65%	0.55
OML	1.12	0.82	22%	0.76

Table 3 Kincaid data set. Summary of performance measures for maximum arcwise concentrations.

	Nmse	Cor	fa2	Fb
the presented model	0.74	0.36	66%	0.16
HPDM	0.75	0.44	56%	0.19
OML	1.24	0.15	55%	0.14

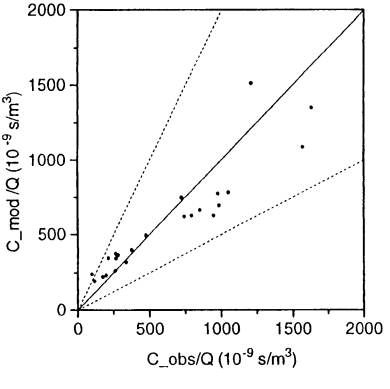

Figure 1 Copenhagen dataset. Comparison of predicted and observed for the tha arcwise maxima concentration. Data between dashed lines are in fa2.

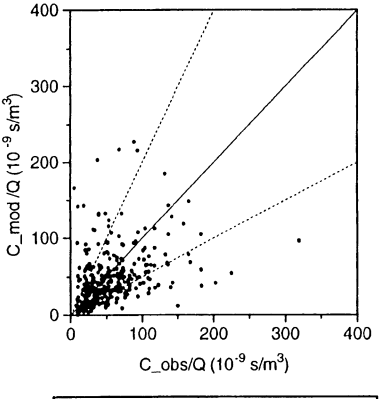

Figure 2 Kincaid dataset. Comparison of predicted and observed for the tha arcwise maxima concentration. Data between dashed lines are in fa2.

The fractional bias is positive in both cases indicating a general underprediction of the model respect to data, i.e. an overprediction of dispersion parameters, more accentuated in the buoyant case. In the last case because of presence of buoyancy it's more difficult to isolate the behaviour of the dispersion parameters as proposed here.

4 Conclusions

A general formulation for the dispersion parameters in a PBL 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 function of similarity coordinate, the non dimensional molecular dissipation rate and the frequency of spectral peaks. The derived multiple dispersion parameters can be applied all atmospheric conditions without discontinuities. The main advantage of the new method consists in the eliminating the necessity of dispersion parameterizations fitting from diffusion experiments. An evaluation of the dispersion parameters was performed by mean of a Gaussian plume model, using experimental ground level concentrations in several atmospheric and experimental conditions. Analysis of the results shows that the dispersion model reproduces adequately the experimental measurements, and in some cases better than other advanced more complex models. Therefore, the presented formulation for the dispersion parameters seems to be suitable for applications in air quality dispersion models.

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