IL NUOVO CIMENTO Vol. 27 C, N. 1 Gennaio-Febbraio 2004
DOI 10.1393/ncc/i2003-10017-5

A model for the estimation of standard deviation of air pollution concentration in different stability conditions

C. Mangia([1]), I. Schipa([1]), G. A. Degrazia([2]), T. Tirabassi([1]) and U. Rizza([1])(*)

([1]) *CNR-ISAC, Institute of Atmospheric Sciences and Climate, 73100 Lecce, Italy*
([2]) *Universidade Federal de Santa Maria, Departamento de Física - Santa Maria, Brazil*

(ricevuto il 21 Luglio 2003; revisionato l' 8 Aprile 2004; approvato il 13 Aprile 2004)

Summary. — We propose to estimate the standard deviations of the air pollution concentration in the horizontal and vertical direction, σ_y and σ_z, based on Pasquill's well-known equation, in terms of the wind variance and the Lagrangian integral time scales, on the basis of an atmospheric turbulence spectra model. The main advantage of the spectral model is its treatment of turbulent kinetic energy spectra as the sum of buoyancy and a shear produced part, modelling each one separately. The formulation represents both shear and buoyant turbulent mechanisms characterizing the various regimes of the Planetary Boundary Layer, and gives continuous values at any elevation and all stability conditions from unstable to stable. As a consequence, both the wind variance and the Lagrangian integral time scales in the dispersion parameters are more general than those found in literature, because they are not derived from diffusion experiments as most parameterizations. Furthermore, they provide a formulation continuous for the whole boundary layer resulting more physically consistent. The σ_y, σ_z parameters, included in a Gaussian model have been tested and compared with a dispersion scheme reported in the literature, using experimental data in different emission conditions (low and tall stacks) and in several meteorological conditions ranging from stable to convective. Results show that the dispersion model with the sigmas parameterisation included, produces a good fitting of the measured ground-level concentration data in all the experimental conditions considered, performing slightly better than other state-of-art models.

PACS `92.60.Sz` – Air quality and air pollution.

1. – Introduction

The Gaussian approach is widely used in the field of air pollution studies to model the statistical properties of the concentration of contaminants emitted in the Planetary Boundary layer (PBL).

(*) E-mail: u.rizza@isac.cnr.it

The conditions under which the mean concentration of a pollutant species emitted from a point source can be assumed to have a Gaussian distribution are highly idealized, since they require stationary and homogeneous turbulence. In the PBL the flow may be assumed quasi-stationary for suitably short periods of time (ca. 10 min to 1h); however, due to the presence of the surface, there are variations with height of both the mean wind and turbulence that cannot always be disregarded.

Much effort has been devoted to the development of non-Guassian models, for handling the non-homogeneous structures of PBL turbulence. However, they still result in excessively large computer runs, either for emergency response applications or for calculating concentration time series over a long time (*e.g.*, a year). The latter are especially important in the evaluation of violations of air pollution standards, which are often expressed in high percentiles.

Conversely, Gaussian models are fast, simple, do not require complex meteorological input, and describe the diffusive transport in an Eulerian framework, making easy use of the Eulerian nature of measurements.

For these reasons they are still widely used by the environmental agencies all over the world for regulatory applications. However, because of their well-known intrinsic limits, the reliability of a Gaussian model strongly depends on the way the dispersion parameters are determined on the basis of the turbulence structure of the PBL and the model's ability to reproduce experimental diffusion data. A great variety of formulations exist [1-7]. Most of them are based on the approach proposed by Pasquill [8], which retained the essential features of Taylor's statistical theory, but evaluated the dispersion parameters in terms of the turbulence quantities and their related time scale, using the following expression:

$$\sigma^2 = \left(\overline{u'^2}\right) T^2 F(T, T_\mathrm{L}) \,, \tag{1}$$

where $\left(\overline{u'^2}\right)$ is the wind velocity variance, T_L is the related Lagrangian integral time scale, T is the travel time and F is a universal function.

Usually, the wind variances are scaled following the similarity theory on the basis of the experimental wind data [9, 10]. The Lagrangian time scales are often parameterized as constant (in the case of the lateral time scale $T_{\mathrm{L}v}$), or as empirical functions of basic boundary layer parameters (in the case of vertical time scale $T_{\mathrm{L}w}$) [1, 4, 6, 8, 11]. Often they give different results for the same atmospheric stability, as well as discontinuities at the transition of the various stability regimes.

An approach for estimating turbulence parameters as a function of atmospheric spectra for all stability conditions of PBL has recently been derived by Degrazia *et al.* [12]. It is based on Taylor's statistical theory, the observed turbulence spectral properties and the observed characteristics of energy containing eddies. In the present study, we utilize this approach to determine an analytical expression for the dispersion parameters to be used in a Gaussian model in different meteorological and emission scenarios.

2. – Dispersion parameters

The starting point of the proposed approach is Taylor's (1921) classical dispersion theory [13], where the mean-square displacement of particles moving in a turbulent field can be expressed as a function of travel time T:

$$\sigma^2(T) = 2\int_0^T \int_0^t \overline{u'(t)u'(t+\xi)}\mathrm{d}\xi\mathrm{d}t\,, \tag{2}$$

where u' is the turbulent velocity at a given time and the overbar represents ensemble-averaging.

In a stationary and homogeneous turbulent flow, eq. (2) can be expressed in terms of the normalised Lagrangian autocorrelation function $\rho_\mathrm{L}\,(t)$

$$\sigma^2(T) = \overline{u'^2}\int_0^T \int_0^t \rho_\mathrm{L}(t)\mathrm{d}t\,, \tag{3}$$

where $\overline{u'^2}$ represents the Lagrangian variance of the turbulent wind field, which is assumed equivalent to the Eulerian one, following [14].

In order to overcome the practical difficulties relating to the knowledge of the Lagrangian autocorrelation function, which is ideally extended over the entire range of time, Pasquill [8] suggested a method that retained the essential character of Taylor's statistical features, but was much more amenable to parameterization in terms of readily measured quantities.

He considered the two asymptotic travel time limits. For small travel diffusion time T, the correlation function $\rho_\mathrm{L}(t)$ is close to unity, so eq. (3) becomes

$$\sigma^2(T) = \overline{u'^2}T^2\,. \tag{4}$$

For large travel time T (*i.e.* for a travel time bigger than the Lagrangian decorrelation time scale), the particle velocities are expected to be uncorrelated with initial velocity, so $\rho_\mathrm{L}(t) \to 0$ and eq. (3) can be written as

$$\sigma^2(T) = 2\overline{u'^2}\left(\int_0^\infty \rho_\mathrm{L}(t)\mathrm{d}t\right)T = 2\overline{u'^2}TT_\mathrm{L}\,. \tag{5}$$

The interpolation between the two extreme limits (eqs. (4) and (5)) leads to eq. (1), that is

$$\sigma^2 = \left(\overline{u'^2}\right)T^2F(T,T_\mathrm{L})\,.$$

The exact form of the function F is determined from experimental data in order to compensate any deviations from homogeneous and stationary conditions that are inherent in the assumed Gaussian distribution [15].

Different forms for F can be found in the literature: they are mainly expressed as $\left(\frac{1}{1+\gamma T/T_\mathrm{L}}\right)$, with different constant γ for lateral and vertical directions, and for stability conditions.

One of the most used empirical forms for the lateral (σ_y) and vertical (σ_z) dispersion parameter is given by [3, 11, 16, 17]

$$\sigma^2 = \overline{(u'^2)}\, T^2 \frac{1}{(1 + 0.5T/T_{\mathrm{L}})} \,. \tag{6}$$

Using this formulation and determining $\overline{u'^2}$, T_{L} as a function of turbulence spectra with the following expressions:

$$\overline{u'^2} = \int_0^\infty S^{\mathrm{E}}(n)\mathrm{d}n \,, \tag{7}$$

where $S^{\mathrm{E}}(n)$ is the Eulerian spectrum of energy, and

$$T_{\mathrm{L}} = \frac{\beta F^{\mathrm{E}}(0)}{4} \,, \tag{8}$$

where $F^{\mathrm{E}}(0)$ is the value of the normalised Eulerian energy spectrum at $n = 0$, β is the ratio of the Lagrangian to the Eulerian integral time scales of turbulent field given by [18]

$$\beta = \left(\frac{\pi}{16} \frac{\overline{u}}{\overline{u'^2}} \right)^{1/2} \,, \tag{9}$$

where $\overline{u}$ is the mean horizontal wind speed.

Therefore, in the present context the main problem concerns the determination of a realistic wind turbulent spectra valid for any stability condition. A model for turbulence spectra for all atmospheric conditions has been derived in the previous papers [12, 19, 20]. It represents both shear and buoyant mechanisms and gives continuous values with height for any stability conditions.

2·1. *Unstable case.* – For the unstable boundary layer, we assume the hypothesis of superposition of the effects produced by the two forcing mechanisms, thermal and mechanical. Thus, we can write the dimensional Eulerian spectra as

$$S^{\mathrm{E}}(n) = S^{\mathrm{E}}_{\mathrm{c}}(n) + S^{\mathrm{E}}_{\mathrm{m}}(n) \,, \tag{10}$$

where the first term on the right represents the buoyancy-produced part, the second is the mechanical component, and the subscripts “c” and “m” are for convective and mechanical terms, respectively.

Assuming that total turbulent energy can be expressed as the sum of the convective and mechanical parts, and working on the hypothesis that mechanical and convective velocities are uncorrelated, we arrive at the separation of eq. (2) into two independent parts, convective and mechanical

$$\sigma^2 = \sigma^2_{\mathrm{c}} + \sigma^2_{\mathrm{m}} \,, \tag{11}$$

with

$$\sigma_{\mathrm{c}}^2(T) = 2\int_0^T \int_0^t \overline{u'_{\mathrm{c}}(t)u'_{\mathrm{c}}(t+\xi)}\mathrm{d}\xi\mathrm{d}t\,, \tag{12a}$$

$$\sigma_{\mathrm{m}}^2(T) = 2\int_0^T \int_0^t \overline{u'_{\mathrm{m}}(t)u'_{\mathrm{m}}(t+\xi)}\mathrm{d}\xi\mathrm{d}t\,. \tag{12b}$$

Therefore, eq. (6) can be split into two terms:

$$\sigma_{\mathrm{c}}^2 = \overline{u_{\mathrm{c}}'^2}T^2\frac{1}{(1+0.5T/T_{\mathrm{Lc}})}\,, \tag{13a}$$

$$\sigma_{\mathrm{m}}^2 = \overline{u_{\mathrm{m}}'^2}T^2\frac{1}{(1+0.5T/T_{\mathrm{Lm}})}\,. \tag{13b}$$

For the vertical direction, the convective terms are [12, 20]

$$\frac{nS_{w\mathrm{c}}^{\mathrm{E}}(n)}{w_*^2} = \frac{0.98c_w f}{(f_w q_{w\mathrm{c}})^{5/3}\left[1+1.5\frac{f}{(f_w q_{w\mathrm{c}})}\right]^{5/3}}(\Psi_{\varepsilon\mathrm{c}})^{2/3}\left(\frac{z}{h}\right)^{2/3}, \tag{14a}$$

$$\overline{w_{\mathrm{c}}'^2} = 0.6\frac{(z/h)^{2/3}}{q_{w\mathrm{c}}^{2/3}}w_*^2\,, \tag{14b}$$

$$F_{w\mathrm{c}}^{\mathrm{E}}(0) = \frac{z}{f_w q_{w\mathrm{c}}\overline{u}}\,, \tag{14c}$$

$$T_{\mathrm{L}w\mathrm{c}} = 0.31\frac{h}{w_*}\left[1-\exp\left[\frac{-4z}{h}\right]-0.0003\exp\left[\frac{8z}{h}\right]\right]^{2/3}, \tag{14d}$$

where w_* is the convective velocity scale, h is the convective boundary layer height, f_w is the spectral peak in neutral condition, $q_{w\mathrm{c}}$ is the stability function and $\Psi_{\varepsilon\mathrm{c}} = \varepsilon_{\mathrm{c}}h/w_*^3$ is the adimensional dissipation rate function, with ε_{c} the buoyant rate of Turbulent Kinetic Energy (TKE) dissipation.

The respective mechanical terms are given by [12, 20]

$$\frac{nS_{w\mathrm{m}}^{\mathrm{E}}(n)}{u_*^2} = \frac{1.5c_w f}{(f_w)^{5/3}\left[1+\frac{1.5f^{5/3}}{(f_w)^{5/3}}\right]}\Phi_{\varepsilon\mathrm{m}}^{2/3}\,, \tag{15a}$$

$$\overline{w_{\mathrm{m}}'^2} = 1.94\left(1-\frac{z}{h}\right)^2 u_*^2\,, \tag{15b}$$

$$F_{w\mathrm{m}}^{\mathrm{E}}(0) = \frac{0.64z}{f_w\overline{u}}\,, \tag{15c}$$

$$T_{\mathrm{L}w\mathrm{m}} = \frac{0.15z}{(1-z/h)u_*}\,, \tag{15d}$$

where f is the reduced frequency $f = nz/\overline{u}$, u_* is the friction velocity, and the dissipation rate $\Phi_{\varepsilon\mathrm{s}} = \varepsilon_{\mathrm{s}}kz/u_*^3$ is adimensionalized with surface layer scaling parameters; ε_{s} is the mechanical rate of TKE dissipation. The values of constants c_i, of (f_i), q_i, ε_{c} and ε_{s} are found in the appendix.

The further assumption adopted here is that turbulence is estimated at the height z of the plume centroid, H_{eff} [5]:

$$\begin{aligned} &z = H_{\mathrm{eff}} \qquad \text{for} \quad H_{\mathrm{eff}} \geqslant \sigma_z\,, \\ &z = \sigma_z \qquad \text{for} \quad H_{\mathrm{eff}} < \sigma_z\,. \end{aligned} \tag{16}$$

For the lateral direction, the convective terms are given by

$$\frac{nS^{\mathrm{E}}_{v\mathrm{c}}(n)}{w_*^2} = \frac{0.98 c_v f}{(f_v q_{v\mathrm{c}})^{5/3}\left[1 + 1.5\frac{f}{(f_v q_{v\mathrm{c}})}\right]^{5/3}} (\Psi_{\varepsilon\mathrm{c}})^{2/3} \left(\frac{z}{h}\right)^{2/3}, \tag{17a}$$

$$\overline{v'^2_{\mathrm{c}}} = 0.38 w_*^2\,, \tag{17b}$$

$$F^{\mathrm{E}}_{v\mathrm{c}}(0) = \frac{z}{f_v q_{v\mathrm{c}} \overline{u}}\,, \tag{17c}$$

$$T_{\mathrm{L}v\mathrm{c}} = 0.27 \frac{h}{w_*} \tag{17d}$$

and the mechanical terms are

$$\frac{nS^{\mathrm{E}}_{v\mathrm{m}}(n)}{u_*^2} = \frac{1.5 c_v f}{(f_v)^{5/3}\left[1 + \frac{1.5 f^{5/3}}{(f_v)^{5/3}}\right]} \Phi^{2/3}_{\varepsilon\mathrm{m}}\,, \tag{18a}$$

$$\overline{v'^2_{\mathrm{m}}} = 3.2 \left(1 - \frac{z}{h}\right)^2 u_*^2\,, \tag{18b}$$

$$F^{\mathrm{E}}_{v\mathrm{m}}(0) = \frac{0.64 z}{f_v \overline{u}}\,, \tag{18c}$$

$$T_{\mathrm{L}v\mathrm{m}} = 0.25 \frac{z}{(1 - z/h) u_*}\,. \tag{18d}$$

2.2. *Stable case*. – Modelling dispersion in a Stable Boundary Layer (SBL), when the shear production term is the only input to the reservoir of turbulent energy, is still a challenge. Assuming windy conditions and weak surface cooling, the turbulence throughout the SBL (in the presence of a negative surface heat flux) is mainly continuous. In this case, the Eulerian spectra can be expressed as a function of local scales.

For the vertical direction, the terms are [12, 20]

$$\frac{nS^{\mathrm{E}}_{w\mathrm{s}}(n)}{u_*^2} = \frac{1.5 c_w f}{(f_w q_{w\mathrm{s}})^{5/3}\left[1 + \frac{1.5 f^{5/3}}{(f_w q_{w\mathrm{s}})^{5/3}}\right]} \Phi^{2/3}_{\varepsilon\mathrm{s}}\,, \tag{19a}$$

$$\overline{w'^2_{\mathrm{s}}} = \frac{1.94 \left(1 - \frac{z}{h}\right)^2 (1 + 3.7 z/\Lambda)^{2/3} u_*^2}{q^{2/3}_{w\mathrm{s}}}\,, \tag{19b}$$

$$F^{\mathrm{E}}_{w\mathrm{s}}(0) = \frac{0.64 z}{f_w q_{w\mathrm{s}} \overline{u}}\,, \tag{19c}$$

$$T_{\mathrm{L}w\mathrm{s}} = \frac{0.15 z}{(1 - z/h)(1 + 3.7 z/\Lambda) u_*}\,, \tag{19d}$$

where h is now the stable boundary layer height, Λ is the local Monin-Obukhov length, $\Lambda = L(1 - z/h)^{(1.5\alpha_1 - \alpha_2)}$, L is the Monin-Obukhov length, and $\alpha_1 = 3/2$ and $\alpha_2 = 1$.

The terms of lateral direction are given by

$$\frac{nS^{\mathrm{E}}_{v\mathrm{s}}(n)}{u_*^2} = \frac{1.5c_v f}{(f_v q_{v\mathrm{s}})^{5/3}\left[1 + \frac{1.5 f^{5/3}}{(f_v q_{v\mathrm{s}})^{5/3}}\right]} \Phi_{\varepsilon\mathrm{s}}^{2/3} , \tag{20a}$$

$$\overline{v'^2_{\mathrm{s}}} = \frac{3.2\,(1 - z/h)^2\, u_*^2}{(1 + 3.7z/\Lambda)^{2/3}} , \tag{20b}$$

$$F^{\mathrm{E}}_{v\mathrm{s}}(0) = \frac{0.64z}{f_v q_{v\mathrm{s}} \overline{u}} , \tag{20c}$$

$$T_{\mathrm{L}v\mathrm{s}} = \frac{0.25z}{(1 - z/h)(1 + 3.7z/\Lambda)u_*} . \tag{20d}$$

The wind variance and the Lagrangian integral time scales derived by this approach are expressed in terms of the fundamental boundary layer parameters. In contrast to the existing approaches, they are derived as a function of the atmospheric turbulence and do not use information from diffusion experiments, so they can be considered more general. Furthermore, being based on continuous values of the turbulence spectrum, the turbulence parameters provide continuous values in the PBL at any elevation and in stability conditions ranging from convective to stable, resulting more physically correct. Taylor's statistical diffusion theory being strictly valid only for homogeneous turbulence, eqs. (17)-(20) employing a velocity spectrum dependent on height z, can be extended to model the case of inhomogeneous turbulence [12].

3. – The Gaussian model

According to the Gaussian plume model, if the wind is along the x-direction, the ground level concentration can be given by

$$c(x, y, 0) = \frac{Q}{\pi \overline{u} \sigma_y \sigma_z} \exp\left[-0.5\left(\frac{H_{\mathrm{eff}}}{\sigma_z}\right]^2\right) \exp\left[-0.5\left(\frac{y}{\sigma_y}\right]^2\right) + R_{\mathrm{s}} , \tag{21}$$

where Q is the source strength, H_{eff} is the *effective* plume height given by $H_{\mathrm{eff}} = H_{\mathrm{s}} + \Delta H$, where H_{s} is the geometric source height, and ΔH is the plume rise, R_{s} are the terms associated to reflection from the top of the mixing layer, taken into account by the introduction of imaginary sources.

The ground-level crosswind-integrated concentration is defined as

$$Cy = \int_{-\infty}^{\infty} C(x, y, 0)\mathrm{d}y . \tag{22}$$

3$\cdot$1. *Wind profile*. – The wind speed profile used has been parameterised following the similarity theory of Monin-Obukhov and the OML model [5]:

For $L < 0$

$$\overline{u}(z) = \frac{u_*}{k}[\ln(z/z_0) - \Psi_\mathrm{m}(z/L) + \Psi_\mathrm{m}(z_0/L)] \qquad \text{if } z \leqslant z_\mathrm{b}\,, \tag{23a}$$

$$\overline{u}(z) = \overline{u}(z_\mathrm{b}) \qquad \text{if } z > z_\mathrm{b}\,, \tag{23b}$$

where $z_\mathrm{b} = \min[|L|, 0.1h]$, z_0 is the roughness length and Ψ_m is a stability function given by

$$\Psi_\mathrm{m} = 2\ln\left[\frac{1+A}{2}\right] + \ln\left[\frac{1+A^2}{2}\right] - 2\tan^{-1}(A) + \frac{\pi}{2} \tag{24}$$

with

$$A = (1 - 16z/L)^{1/4}\,, \tag{25}$$

$k = 0.4$ is the Von Karman constant.

For $L > 0$

$$\overline{u}(z) = \frac{u_*}{k}[\ln(z/z_0) + \Psi_\mathrm{m}(z/L)]\,, \tag{26}$$

where in this case the function Ψ_m is given by

$$\Psi_\mathrm{m}\left(\frac{z}{L}\right) = 4.7\left(\frac{z}{L}\right)\,. \tag{27}$$

3˙2. *Plume rise*. – The algorithm for calculating the plume rise includes models suggested by Briggs separately for unstable, neutral and stable conditions [21]. Here, we mention only the final results. For more details, the reader is referred to the original paper by Briggs [21] or to the report by Weil and Brower [22].

In convective or neutral conditions the effective height is given by either of two models, the "break up" model or the "touch down" model.

Final rise for the "break up" formulation occurs when the turbulent dissipation rate inside the plume decreases to that of the surrounding turbulent environment. Thus, the final plume rise formula is given by

$$\Delta H = 4.3\left(\frac{f_\mathrm{b}}{u_\mathrm{s} w_*^2}\right)^{3/5} H_\mathrm{s}^{2/5}\,, \tag{28}$$

where f_b is the buoyancy flux and u_s is the wind speed at the source height.

The "touch down" model assumes that in strongly convective conditions a plume is eventually brought to ground by the large-scale downdrafts in the CBL

$$\Delta H = 1.0\left(\frac{f_\mathrm{b}}{0.4 u_\mathrm{s} w_*^2}\right)\left(1 + 2\frac{H_\mathrm{s}}{\Delta H}\right)\,. \tag{29}$$

Equation (29) is solved iteratively for ΔH.

TABLE I. – *Main characteristics of the three experiments.*

Experiment	H_s (m)	u_* range (m s^{-1})		h/L range		Distance from the source (m)		Measured data
Copenhagen	115	0.36	1.05	−444	−33	2000	6000	Cy, Cmax
Prairie Grass	1.5	0.05	0.60	−212.0	7.2	50	800	Cy
Kincaid	187	0.2	1.04	−551	25	1000	50000	Cmax

In neutral stability, Briggs' break-up model predicts the final plume rise to be

$$\Delta H = 1.3 \left(\frac{f_b}{u_s u_*^2} \right) \left(1 + \frac{H_s}{\Delta H} \right)^{2/3} . \tag{30}$$

Equation (30) is solved iteratively for ΔH.

The three final rise formulas were obtained for different limiting conditions and interpolation formulas were not given for "in between" conditions. Following the procedure indicated by Briggs [21] the formula giving the lowest plume rise is chosen.

In stable conditions we have

$$\Delta H = 2.6 \left(\frac{f_b}{u_s s} \right)^{1/3} , \tag{31}$$

where s is the stability parameter

$$s = \frac{g}{T_a} \frac{\partial \theta}{\partial z} ,$$

$\partial\theta/\partial z$ is the potential temperature gradient, T_a the air ambient temperature and g the gravity acceleration. Following [23] we use as a default approximation $\partial\theta/\partial z$ taken as 0.02 Km^{-1} for $1/L < 0.35$ and $\partial\theta/\partial z = 0.035$ Km^{-1} for $1/L \geqslant 0.35$.

4. – Field experiments

The parameterisations for dispersion coefficients have been evaluated through the Gaussian model using three experimental datasets with different emission and meteorological scenarios, so that the evaluation covered most of the turbulent regimes as described in [24, 25].

The Copenhagen field campaign [26] took place in the suburbs of Copenhagen in 1978. A SF_6 tracer was released without buoyancy from a tower at a height of 115 m, and collected at ground level on arcs located around 2000, 4000 and 6000 meters from the release point. The site was mainly residential with a roughness length, z_0, of 0.6 m. The meteorological conditions during the dispersion experiments ranged from moderately unstable to convective.

The Prairie Grass dataset [27] consists of dispersion data from a field experiment conducted in open country (z_0 was 0.008 m) during the summer of 1956 in O'Neill, Nebraska. Sulphur dioxide was released from a continuous point source at the height of

0.46 m and collected by 5 arcs, 50, 100, 200, 400, 800 meters from the source. Here, we use the values of the crosswind-integrated concentrations, as calculated and reported by [28, 29].

The Kincaid dataset [30] is a part of the EPRI Project, Plume Model Validation and Development. The power plant, located in Illinois (USA), is surrounded by flat farmland with some lakes. During the experiment, SF_6 was released with buoyancy from a 187 tall stack and recorded on a network consisting roughly of 1800 samplers (200 of which were active every hours) on arcs, whose distance from the source ranged from 1 to 50 km. Ground level concentration patterns are quite irregular, with high concentration values found close to low values; thus, neither of the plumes have the regular structure that a Gaussian model assumes. Therefore, the evaluation presented here is focused on the model's capability to predict the maxima concentrations in the different turbulent regimes where the maximum of the observed concentration on an arc of monitoring stations is interpreted as being the centreline concentration.

The hypothesis of large travel time was verified for each run of the experiment, comparing the tracer travel time with the decorrelation time scale T_w, determined following the approach suggested by [12]. Table I presents a summary of significant meteorological and experimental conditions.

5. – Model evaluation

The proposed σ_y and σ_z formulation (hereafter MODEL I) was evaluated utilizing experimental data, and compared with a scheme based on similarity theory and the micrometeorological variables proposed by Irwin [31] (hereafter MODEL II), which is included in several regulatory models

$$\sigma_y = \left(\overline{v'^2}\right)^{1/2} T F_y(T, T_{\mathrm{L}v}) , \tag{32}$$

$$\sigma_z = \left(\overline{w'^2}\right)^{1/2} T F_z(T, T_{\mathrm{L}w}) , \tag{33}$$

with

$$F_y = \left[1 + 0.9(T/1000)^{1/2}\right]^{-1} , \tag{34}$$

$$F_z = \left[1 + 0.9(T/500)^{1/2}\right]^{-1} \qquad L < 0 , \tag{35a}$$

$$F_z = \left[1 + 0.945(T/100)^{0.806}\right]^{-1} \qquad L > 0 . \tag{35b}$$

Figures 1-3 show the scatter diagrams between the measured and predicted concentration data using the two $\sigma_y - \sigma_z$ schemes for the three datasets utilised. The two models are indicated by different symbols. Table II presents some performance measurements, obtained using the statistical evaluation procedure described by [32] and defined in the following way:

nmse (normalised mean square) = $\overline{(C_{\mathrm{m}} - C_{\mathrm{p}})^2}/\overline{C_{\mathrm{m}}C_{\mathrm{p}}}$,
cor (correlation)= $\overline{(C_{\mathrm{m}} - \overline{C_{\mathrm{m}}})(C_{\mathrm{p}} - \overline{C_{\mathrm{p}}})}/\sigma_{\mathrm{m}}\sigma_{\mathrm{p}}$,
fa2 = $C_{\mathrm{p}}/C_{\mathrm{m}} \in [0.5, 2]$,

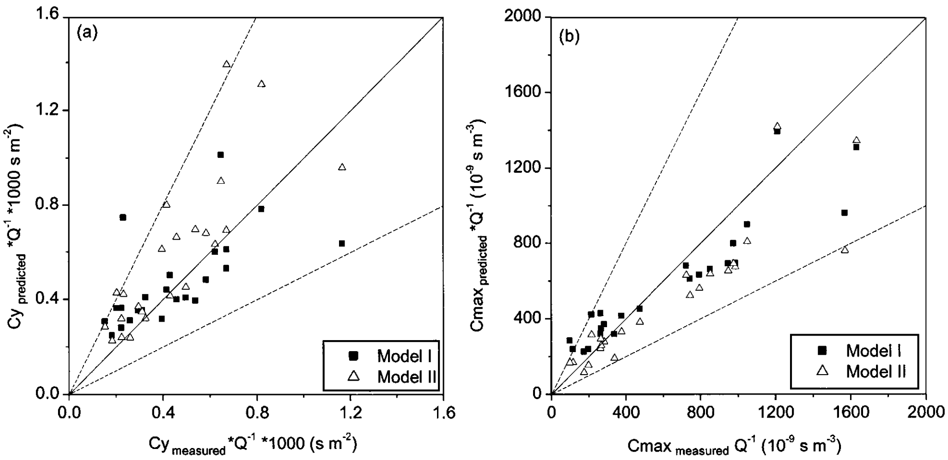

Fig. 1. – Copenhagen field experiments. Scatter plot between measured and predicted concentration data. Data between dashed lines correspond to ratio $C_{\mathrm{predicted}}/C_{\mathrm{measured}} \in [0.5, 2]$. a) Crosswind-integrated concentration; b) arcwise maximum concentration. Model I is given by using the model proposed. Model II is Irwin's scheme.

fb (fractional bias)= $\left(\overline{C_{\mathrm{m}}} - \overline{C_{\mathrm{p}}}\right) / \left(0.5\left(\overline{C_{\mathrm{m}}} + \overline{C_{\mathrm{p}}}\right)\right)$,
where the subscripts "m" and "p" refer to measured and predicted quantities, respectively, and an overbar indicates an average.

Both models adequately reproduce the experimental concentration data in the various stability regimes, and when emission is close to the ground and/or elevated. Most of the predictions from Model I are in a factor of two of the measurements, and correlation is quite good for Copenhegen and Prairie Grass experiments. A large scatter is evident

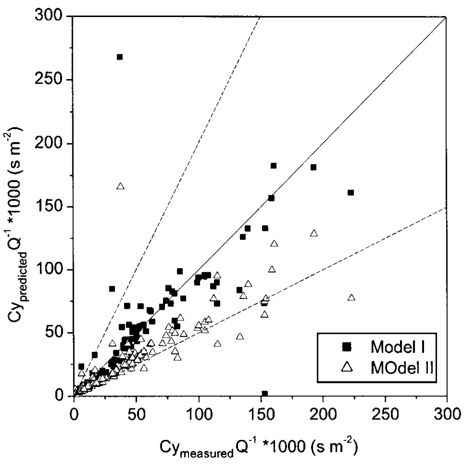

Fig. 2. – Prairie Grass experiments. Scatter plot between measured and predicted crosswind-integrated concentrations. Data between dashed lines correspond to ratio $C_{\mathrm{predicted}}/C_{\mathrm{measured}} \in [0.5, 2]$. Model I is given by using the model proposed. Model II is Irwin's scheme.

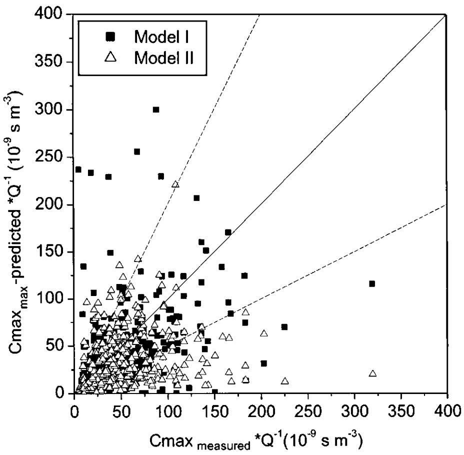

Fig. 3. – Kincaid dataset. Scatter plot between measured and predicted arcwise maximum concentration data. Data between dashed lines correspond to ratio $C_{\mathrm{predicted}}/C_{\mathrm{measured}} \in [0.5, 2]$. Model I is given by using the model proposed. Model II is Irwin's scheme.

Table II. – *Statistical evaluation of models results.* "Cy" *indicates the crosswind-integrated concentration;* "Cmax" *indicates the arcwise maximum concentration.*

Copenhagen dataset				
	nmse	Cor	Fa2	Fb
Cy				
Model I	0.13	0.74	0.96	0.03
Model II	0.12	0.79	0.96	−0.07
Cmax				
Model I	0.11	0.93	0.91	−0.08
Model II	0.18	0.90	0.96	−0.22
Prairie Grass dataset				
	nmse	Cor	Fa2	Fb
Cy				
Model I	0.46	0.82	0.91	−0.07
Model II	0.87	0.85	0.83	−0.47
Kincaid dataset				
	nmse	Cor	Fa2	Fb
Cmax				
Model I	0.86	0.37	0.66	−0.18
Model II	1.21	0.19	0.48	−0.42

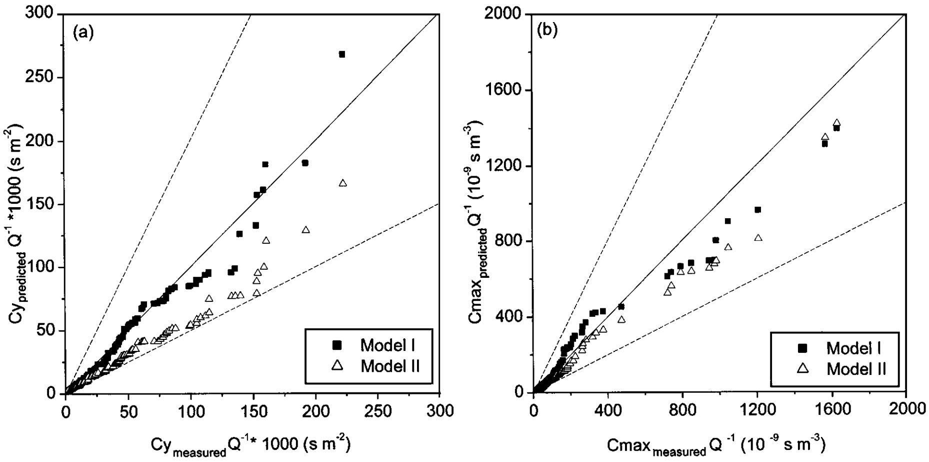

Fig. 4. – Comparison of predicted and observed concentration data paired with respect to their rank. Data between dashed lines correspond to ratio $C_{\mathrm{predicted}}/C_{\mathrm{measured}} \in [0.5, 2]$. a) Crosswind-integrated concentration; b) arcwise maximum concentration. Model I is given by using the model proposed. Model II is Irwin's scheme.

for the Kincaid dataset, this can be due to the non-correct estimation of the wind and temperature profile which can cause a wrong plume rise determination and to the complex concentration patterns difficult to reproduce with a Gaussian model. Overall, the results obtained are similar to those found from other state-of-the-art models [33].

From a regulatory point of view, it is usually only required that a model properly predicts the frequency distribution of concentration. In figs. 4a and b, the predicted and observed concentrations are paired with respect to their rank order. Thus, observations are not matched in time or in space.

In general, the figures show a good agreement for the model proposed, whereas Model II shows a general tendency to under-predict measured data. This is also confirmed by the fractional bias, which is always negative and higher for Model II with respect to the model described here. Table II evidences also a poor performance of Model II for Kincaid data set: all the statistical indexes are worse as respect as Model I.

Table III summarises the values for the performance measures for other state-of-the-art models in their evaluation with Copenhagen, Prairie Grass and Kincaid datasets. It is not easy to interpret the statistical indexes given in this table, because some of the data sets have been used for some models during model development. As consequence, the validation exercise does not constitute an independent test of such models.

Values for Copenhagen were obtained as part of a model validation exercise during the Workshop on Operational Short-range Atmospheric Dispersion Models for Environmental Impact Assessment in Europe [33], they refer to OML model [5] which is a regulatory model used in Denmark. Values for Kincaid and Prairie Grass are derived from Hanna [34] and they regard the models ADMS [35] and AERMOD [36] which are new state-of-art dispersion models recently proposed for use in regulatory applications in the United Kingdom and the United States, respectively. OML is a Gaussian-type model for all stability conditions both for y- and z-directions, while ADMS and AERMOD assume a bimodal distribution of turbulent vertical velocities for convective conditions, so the

TABLE III. – *Model evaluation results for Model I, OML, ADMS and AERMOD for the three experiments.* "Cy" *indicates the crosswind-integrated concentration;* "Cmax" *indicates the arcwise maximum concentration.*

Copenhagen dataset				
	nmse	Cor	Fa2	Fb
Cy				
Model I	0.13	0.74	0.96	0.03
OML	0.52	0.89	0.56	0.57
Prairie Grass dataset				
	nmse	Cor	Fa2	Fb
Cy				
Model I	0.46	0.82	0.91	−0.07
ADMS 3	0.88	0.89	0.61	0.19
AERMOD	1.87	0.75	0.76	0.00
Kincaid dataset				
	nmse	Cor	Fa2	Fb
Cmax				
Model I	0.86	0.37	0.66	−0.18
OML	1.24	0.15	0.55	0.14
ADMS 3	0.60	0.45	0.67	0.05
AERMOD	2.10	0.40	0.29	0.59

vertical concentration distribution is skewed in Gaussian in convective conditions, while is assumed Gaussian in neutral and stable atmosphere. All the models assume a Gaussian distribution in the crosswind horizontal direction for all stabilities. Comparison between the statistical indexes indicates a general better performance of Model I with respect to similar Gaussian model (*i.e.* Model II and OML). Concerning the Prairie Grass experiment, Model I is shown to give better performance than the other models in terms of nmse and fraction within a factor of 2. The fb is zero for AERMOD, but this is because the Prairie Grass results have been used directly in the AERMOD formulation, with the original formulation being modified to take these into account for surface sources. For Kincaid data set results obtained with Model I are comparable with ADMS model.

The results and the relative statistics highlight a rather satisfactory performance of the model proposed in all of the experiments considered, with respect to other state-of-art models which include more complex algorithms for concentration distribution, plume rise and micrometeorological parameters.

6. – Conclusions

The authors have presented a model for vertical and lateral dispersion parameters, for use in a PBL Gaussian model and for a wide range of atmospheric stability conditions.

The model proposed is based on Taylor's statistical diffusion theory, and further developments due to Pasquill. Employing the empirical relationship between stability and wavelength peak for the turbulent kinetic energy spectra, the turbulence dispersion parameters are expressed in terms of the energy-containing eddies, which are mainly responsible for the turbulent transport processes in the PBL. The assumption of continuous turbulence spectra and variances allows the parameterizations to be continuous in the PBL at all elevations, and in stability conditions ranging from convective to neutral, and from neutral to stable, so that a simulation of a full diurnal cycle becomes possible. It represents a step forward with respect to the previous works presented by the authors [19, 37], the dispersion parameters being expressed in analytical form and valid for all stability conditions and source heights. In addition, the model allows to overcome the discretization of the PBL into different turbulent regimes, as well as possible jumps at the boundaries of these regimes, which are typical of existing models.

The dispersion parameters are included in a Gaussian model, and compared with a widely used scheme in several turbulent regimes in different emission scenarios, using different experimental concentration data. Analysis of results and relative statistical analysis show that the model produces a good fit for the experimental ground level concentration data in the various stability regimes identifying the PBL, when emissions are either close to ground or elevated.

The improvement consists essentially in the fact that the turbulent parameters used in the sigmas formulations are not derived from diffusion experiments, they are continuous at all elevations and for stability regimes, resulting more general and physically consistent.

The results obtained are promising as to the utilization of the new formulation in applications for regulatory air pollution modelling.

Appendix

The values of constants are:

– $c_v = c_w = 0.4$;

– $f_v = 0.16 \quad f_w = 0.35$;

– $q_{wc} = \left| \begin{array}{ll} 0.48 & z \leq 0.1\ h \\ 1.6\ z/h(1. - e^{-4z/h} - 3.10^{-4} e^{8z/h})^{-1} & 0.1\ h \leq z \leq h \end{array} \right|$;

– $q_{ws} = 1 + 3.7 \left(\frac{z}{\Lambda} \right)$;

– $q_{vc} = 4.16 \frac{z}{z_i}$;

– $q_{vs} = 1 + 3.7 \left(\frac{z}{\Lambda} \right)$.

The buoyancy/shear ensamble average rates of dissipation of TKE are:

– $\epsilon_{\rm c} = 0.4\dfrac{w_*^3}{h}$;

– $\epsilon_{\rm s} = \dfrac{u_*^3}{kz}\left(1 - \dfrac{z}{h}\right)\phi_{\rm m}$;

– $\phi_{\rm m} = (1 - 15z/L)^{-1/4}$.

REFERENCES

[1] Hanna S. R., Briggs G. A., Deardoff J., Egan B. A., Gifford F. A. and Pasquill F., *Bull. Am. Meteorol. Soc.*, **58** (1977) 1305.
[2] Bowen B. M., *J. Appl. Meteorol.*, **33** (1994) 1236.
[3] Briggs G. A., *J. Climate Appl. Meteorol.*, **24** (1985) 1167.
[4] Hanna S. R., *J. Climate Appl. Meteorol.*, **25** (1986) 1426.
[5] Berkowicz R., Olesen H. R. and Torp U., *Proc. NATO-CCMS 16th International Meeting on Air Pollution Modelling and Its Applications*, edited by De Wispelaere C., Schiermeier F. A. and Gillani N. V. (Plenum Press, New York, N.Y. (USA)) 1986, pp. 453-481.
[6] Erbrink J. J., *Bound.-Layer Meteorol.*, **74** (1995) 211.
[7] Mohan M. and Siddiqui T. A., *Bound.-Layer Meteorol.*, **84** (1997) 177.
[8] Pasquill F., *Q. J. R. Meteorol. Soc.*, **97** (1971) 369.
[9] Hanna S. R., *Applications in Air Pollution Modelling*, in *Atmospherice Turbulence and Air Pollution Modelling* (Nieuwstadt and Van Dop) 1982, pp. 275-310.
[10] Hicks B. B., *J. Climate Appl. Meteorol.*, **24** (1985) 607.
[11] Draxler R. R., *Atmos. Environ.*, **10** (1976) 99.
[12] Degrazia G. A., Anfossi D., Carvalho J. C., Mangia C., Tirabassi T., Campos Velho H. F., *Atmos. Environ.*, **34** (2000) 3575.
[13] Taylor G. I., *Proc. London Math. Soc.*, **20** (1921) 196.
[14] Hay J. S. and Pasquill F., *Adv. Geophys.*, **6** (1959) 345.
[15] Seinfield J. H. and Pandis S. N., *Atmospheric Chemistry and Physics* (John Wiley & Sons) 1997.
[16] Gryning S. E. and Lyck E., *J. Climate Appl. Meteorol.*, **23** (1984) 651
[17] Venkatram A. and Wyngaard J. C. (Editors), *Lectures on Air Pollution Modeling* (American Meteorological Society, 45 Beacon Street, Boston, MA) 1988.
[18] Wandel C. F. and Kofoed-Hansen O. O., *J. Geophys. Res.*, **67** (1962) 3089.
[19] Mangia C., Degrazia G. A. and Rizza U., *J. Appl. Meteorol.*, **39** (2000) 1913.
[20] Mangia C., Moreira D. M., Schipa I., Degrazia G. A., Tirabassi T. and Rizza U., *Atmos. Environ.*, **36** (2002) 67.
[21] Briggs G. A., *Atmospheric Science and power production*, DOE/TIC 27601, Dept. of Commerce, Springfield, USA (1984).
[22] Weil J. C. and Brower R. P., *J. Air Poll. Control Assoc.*, **34** (1984) 818.
[23] Golder D., *Bound.-Layer Meteorol.*, **29** (1972) 47.
[24] Holtslag A. A. M. and Nieuwstadt F. T. M., *Bound.-Layer Meteorol.*, **29** (1986) 517.
[25] Gryning S. E., Holtstlag A. A. M., Irwin J. S., Sivertsen B., *Atmos. Environ.*, **21** (1987) 79.
[26] Gryning S. E., *Elevated source SF_6-tracer dispersion experiments in the Copenhagen area*, Risoe-R-446 (1981).
[27] Barad M. L., 1958. Project Prairie Grass. Geophysical Research Paper, No. 59, Vols. I and II, GRD, Bedford, MA.
[28] van Ulden A. P., *Atmos. Environ.*, **12** (1987) 2125.
[29] Nieuwstadt F. T. M., *J. Appl. Meteorol.*, **19** (1980) 157.

[30] Bowne N. E. and Londergan R. J., *Overview, results and conclusions for the EPRI plume model validation and development project: plane site*, EPRI report EA-3074 (1981).
[31] Irwin J. S., *J. Climate Appl. Meteorol.*, **22** (1983) 92.
[32] Hanna S. R., *Atmos. Environ.*, **23** (1989) 1385.
[33] Olesen H. R., *Int. J. Environ. Pollution*, **5** (1995) 761.
[34] Hanna S. R., Egan B. A., Purdum J. and Wagler J., *Int. J. Environ. Pollution*, **16** (2001) 301.
[35] CERC Ltd., 1998 *ADMS Technical Specification*, Cambridge Environmental Research Consultants Ltd. Cambridge UK.
[36] Cimorelli A. J., Perry S. G., Venkatram A., Weil J. C., Paine R. J., Wilson R. J., Lee R. F. and Peters W. D., 1998. *AERMOD – Description of Model Formulation*, US EPA Research Triangle Park NC q27711 USA.
[37] Degrazia G. A., *Nuovo Cimento C*, **21** (1998) 345.