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Turbulent dispersion from tall stack in the unstable boundary layer: A comparison between Gaussian and K-diffusion modelling for nonbuoyant emissions(*)

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Summary. — Most air quality dispersion models used for regulatory applications are based on Gaussian and K-diffusion formulations. The reliability of such models strongly depends on how dispersion parameters and eddy diffusivities are computed on the basis of the update understanding of the Planetary Boundary Layer (PBL) meteorology. In this paper, we compare the performances in simulating pollutants released from continuous point source, by using some Gaussian and K-diffusion models with different assumptions concerning the parameterisation of the dispersion processes. Results show that the Gaussian model, in which the dispersion parameters are directly related to spectral peak of turbulence energy, gives the best overall performances. This could be due to a more realistic description of spreading processes occurring into the PBL. This suggests that, in the context of the regulatory applications, this model can give the best combination between ground level concentration estimates and computer requirements.

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1. – Introduction

Atmospheric dispersion is a direct consequence of turbulence in the PBL. It is well known that atmospheric turbulence is generated by two main driving mechanisms: mechanical and convective. The combination between these two forcings generates a continuous set of dispersion regimes. A traditional scheme used to classify these dispersion

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regimes is that one proposed by Holtslag and Nieuwstadt [1]. In that work they identify a discrete number of stability regimes in the PBL. Such regimes are characterised by appropriate velocity and length scales in relation with the structure of dominant dispersive eddies. As a consequence, the dispersion parameters (eddy diffusivities and sigmas) must be modelled in terms of these scales in the framework of similarity theories.

Actually, there are two basic ways of describing turbulent diffusion: the Eulerian and the Lagrangian approaches. The first focuses on the conservation equation for the mean concentration of a pollutant in a fixed reference system, whereas the Lagrangian approach is based on considering the trajectory of marked fluid particles in the flow.

Although atmospheric dispersion is a Lagrangian process, in practical cases all the scaling parameters are measured in a Eulerian framework. In this context, the main approximate theories used for modelling the distribution of pollutants released from continuous point source are based on the K-diffusion first-order closure.

A class of models largely used for regulatory applications are the Gaussian models which assume that concentration distribution is Gaussian in all the directions. In spite of their simple input requirements they produce results that match experimental data as well as any other model, and also they are less expensive in computational time.

The crosswind integrated concentration in a Gaussian model can be written as

$$C_y(x,z) = \frac{Q}{\sqrt{2\pi}\sigma_z U}\left[\exp\left[\frac{(z-H_\mathrm{s})^2}{2\sigma_z^2}\right] + \exp\left[\frac{(z+H_\mathrm{s})^2}{2\sigma_z^2}\right]\right], \tag{1}$$

where σ_z is the vertical spread of the plume, Q is the rate emission, H_s is the effective stack height, U is the mean wind speed, and x, z are the longitudinal and vertical coordinates, respectively.

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 suitable short periods of time (ca. 10 min to 1 h) but, due to the presence of the surface, there are variations with height of both the mean wind and the turbulence that cannot always be disregarded. So, the main difficulty in applying a Gaussian model is to account for the vertical inhomogeneity of the turbulence on the dispersion parameters. The reliability of the model, therefore, strongly depends on the way the dispersion parameters are calculated and on their ability to reproduce experimental diffusion data.

Improved dispersion algorithms in advanced Gaussian models calculate sigmas basically in two ways. In the first approach, dispersion parameters are directly related to the basic physical parameters describing the turbulent state of the PBL on the basis of diffusion experiments [2]. In the second approach dispersion parameters are evaluated directly from the turbulence variances and related timescale [3, 4].

In the K-models it is assumed that turbulent flux is proportional to the gradient of the mean concentration:

$$-\overline{u_i' C'} = K\frac{\partial C}{\partial x_i}, \tag{2}$$

where C is the mean concentration and $\overline{u'C'}$ is the turbulent flux of concentration. The

resulting steady-state advection-diffusion equation can be written as

$$U\frac{\partial C}{\partial x} = \frac{\partial}{\partial x}\left(K_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right), \tag{3}$$

where K_x, K_y and K_z are the eddy diffusivities. The cross-wind integration of eq. (3) (neglecting the longitudinal diffusion) leads to

$$U\frac{\partial C_y}{\partial x} = \frac{\partial}{\partial z}\left(K_z\frac{\partial C_y}{\partial z}\right), \tag{4}$$

subject to the boundary conditions of zero flux at the ground and PBL top.

Several eddy diffusivity profiles can be found in the literature, and for some approximate forms, analytical solutions of eq. (4) exist [5-7].

A new approach in estimating the eddy diffusivity K and dispersion parameters in the unstable boundary layer has been recently proposed by [8-11]. Making use of Taylor's statistical theory and a model for turbulence spectra, this approach relates plume dispersion in an unstable boundary layer directly to the energy containing eddies acting in the layer. Furthermore, in calculating dispersion parameters such formulation does not make use of any fitting of experimental data.

The aim of this paper is to make a comparison among two Gaussian and two K-diffusion modelling for regulatory applications in the case of elevated source, valid only for flat terrain, in an unstable PBL. The new approach will be utilised in both Gaussian and K-models. For comparison purpose two other models have been considered and tested on experimental data. The first one is a Gaussian model with sigmas consistent with the short-range limit of Taylor's statistical theory [12]. The second one is the KappaG model [13] in which both wind and diffusivity follow a power law profile.

2. – Dispersion models

2˙1. *Gaussian model I.* – The dispersion parameters utilised in this model follow a recent approach developed by Demuth [7] and Degrazia *et al.* [8]. In the framework of Taylor's statistical theory and subsequent development by Pasquill and Smith [14], they obtained an expression for dispersion coefficients as a function of spectral distribution of turbulent kinetic energy.

The vertical dispersion parameter obtained is expressed as

$$\frac{\sigma_z^2}{h^2} = \frac{0.093}{\pi}\int_0^\infty \frac{\sin^2(2.96\Psi_\varepsilon^{1/3}Xn')}{(1+n')^{5/3}n'^2}\mathrm{d}n', \tag{5}$$

where $X = xw_*/Uh$, U is the horizontal mean wind speed at the source height ($z =$ 115 m), w_* is the convective velocity scale, h is the height of the convective boundary layer, $\Psi_\varepsilon = \varepsilon h/w_*^3$ is the nondimensional dissipation rate function, ε is the buoyant rate of TKE dissipation and n' is the nondimensional frequency.

The integral form of the dispersion parameter (eq. (5)) is more complicated than the algebraic one available in the literature. On the other hand it is more general since, unlike the algebraic parameterizations, it does not utilize turbulent dispersion measurements. Equation (5) relates plume dispersion in an unstable layer directly and explicitly

to the effective turbulent eddy sizes acting in the layer. Integration of eq. (5) with ordinary methods of numerical analysis is straightforward. Furthermore, the computational requirements are not excessive because the turbulent filter in the integrals allows a reduction in the upper integration limit to a finite value which depends on travel time.

Gaussian model I is then obtained by inserting eq. (5) in eq. (1).

2˙2. *Gaussian model II*. – The Gaussian model II uses the Weil and Brower [12] sigma-scheme which is derived considering the short-range limits of Brigg's curve, consistent with Taylor's statistical theory:

$$\sigma_z = \sigma_w t \,. \tag{6}$$

The vertical wind variance is obtained by fitting data from the Minnesota boundary layer experiment by Kaimal *et al.* [15]:

$$\sigma_w = 0.56 w_* \,; \tag{7}$$

such fitting is valid to the upper 90% of the mixed layer. The resulting vertical dispersion parameter utilised in eq. (1) is

$$\sigma_z = 0.56 w_* \frac{x}{U} \,, \tag{8}$$

where U is the horizontal mean wind speed at the source height ($z = 115$ m).

2˙3. *K-model I*. – The first K-model considered here is proposed by Vilhena *et al.* [16]. This is an analytical model based on a discretization of the PBL in N subintervals in such a manner that inside each interval $K_z(z)$ and $U(z)$ assume the average values

$$K_n = \frac{1}{z_n - z_{n-1}} \int_{z_{n-1}}^{z_n} K_z(z) \mathrm{d}z \,, \tag{9}$$

$$U_n = \frac{1}{z_n - z_{n-1}} \int_{z_{n-1}}^{z_n} U_n(z) \mathrm{d}z \,. \tag{10}$$

Therefore, the solution of eq. (4) is reduced to the solution of N problems of the type

$$U_n \frac{\partial}{\partial x} C_y^n = K_z \frac{\partial^2}{\partial z^2} C_y^n \qquad \text{with} \quad z_{n-1} \leqslant z \leqslant z_n \tag{11}$$

for $n = 1, \ldots, N$, where C_y^n denotes the concentration at the n-th subinterval. To determine the $2N$ integration constants the additional $(2N-2)$ conditions, namely continuity of concentration and flux at the interface, are considered:

$$C_y^n = C_y^{n+1} \,, \qquad n = 1, 2, ..., (N-1) \,, \tag{12}$$

$$K_n \frac{\partial C_y^n}{\partial z} = K_{n+1} \frac{\partial C_y^{n+1}}{\partial z} \,, \qquad n = 1, 2, ..., (N-1) \,. \tag{13}$$

Applying the Laplace transform in eq. (11) gives

$$\frac{\partial^2}{\partial x^2}C_y^n(s,z) - \frac{U_n S}{K_n}C_y^n(s,z) + \frac{U_n}{K_n}C_y^n(0,z) = 0\,, \tag{14}$$

where $C_y^n(s,z) = L\{C_y^n(x,z); x \to s\}$, which has the well-known solution

$$C_y^n(s,z) = A_n e^{-R_n z} + B_n e^{R_n z} + \frac{Q}{2R_a}(e^{-R_n(z-H_s)} - e^{R_n(z-H_s)})\,, \tag{15}$$

where

$$R_n = \pm\sqrt{\frac{U_n S}{K_n}} \qquad \text{and} \qquad R_a = \pm\sqrt{U_n S K_n}\,.$$

Finally, applying the interface and boundary conditions we come out with a linear system for the integration constants. Henceforth the concentration is obtained by inverting numerically the transformed concentration C_y^n by the Gaussian quadrature scheme [17]

$$C_y^n(x,z) = \sum_{j=1}^{M} A_j \frac{P_j}{x}\left(A_n \exp\left[-\sqrt{\frac{P_j U_n}{xK_n}}z\right] + B_n \exp\left[\sqrt{\frac{P_j U_n}{xK_n}}z\right]\right)\,, \tag{16}$$

$$\begin{aligned} C_y^n(x,z) = \sum_{j=1}^{M} A_j \frac{P_j}{x}\left[A_n \exp\left[-\sqrt{\frac{P_j U_n}{xK_n}}z\right] + B_n \exp\left[\sqrt{\frac{P_j U_n}{xK_n}}z\right] + \right. \\ \left. + \frac{1}{2}\frac{Q}{\sqrt{\frac{P_j K_n U_n}{x}}}\left(\exp\left[-(z-H_s)\sqrt{\frac{P_j U_n}{xK_n}}\right] - \exp\left[(z-H_s)\sqrt{\frac{P_j U_n}{xK_n}}\right]\right)\right]\,. \end{aligned} \tag{17}$$

The solution (16) is valid for each layer that does not contain the contaminant source, while eq. (17) must be used to evaluate the concentration field in the layer that contains the pollutant source. In such formulation the ground-level concentration is an average value over the first layer and calculated from eqs. (16) or (17) as $C_y^{n=0}$.

Here A_j and P_j are the weights and roots of the Gaussian quadrature scheme. In this study was considered $N = 8$ because this value provides the desired accuracy with small computational effort. Obviously, the greater the number of layer (N), the more accurate the calculated concentration pattern but with a much more expensive computation time.

The eddy diffusivity profiles utilised in eqs. (16) and (17) are based on Degrazia *et al.* [8]:

$$\frac{K_z}{w_* h} = 0.22\left(\frac{z}{h}\right)^{1/3}\left(1-\frac{z}{h}\right)^{1/3}\left[1 - \exp\left[-\frac{4z}{h}\right] - 0.0003\exp\left[\frac{8z}{h}\right]\right]. \tag{18}$$

The wind speed profile has been parameterised following the OML model [2]:

$$U = \frac{u_*}{\kappa}[\ln(z/z_0 - \Psi_m(z/L) + \Psi_m(z_0/L)]\,, \qquad \text{if} \quad z \leqslant z_b\,, \tag{19}$$

$$U = U(z_b)\,, \qquad \text{if} \quad z > z_b\,, \tag{20}$$

where u_* is the friction velocity, $\kappa = 0.4k$ is the Von Karman constant, z_0 is the roughness length, Ψ_m is a stability function given by [18]

$$\Psi_m = 2\ln\left[\frac{1+A}{2}\right] + \left[\frac{1+A^2}{2}\right] - 2\tan^{-1}A + \frac{\pi}{2}, \tag{21}$$

$$A = (1 - 16z/L)^{1/4}, \tag{22}$$

L is the Monin Obukhov length and $z_b = \min[|L|, 0.1h]$.

2˙4. *K-model II.* – The other analytical model utilised here is the KappaG model developed by Tirabassi *et al.* [13]. It is based on Demuth [7] solution of the advection-diffusion K-equation (eq. (3)) in which both the wind and eddy diffusivity are described in terms of power law profiles, that is

$$u(z) = u_1\left(\frac{z}{z_1}\right)^{\alpha}, \tag{23}$$

$$K(z) = K_1\left(\frac{z}{z_1}\right)^{\beta}, \tag{24}$$

where $z_1 = 10$ m, $u_1 = u(z_1)$, see table I, $K_1 = \frac{\kappa u_* z_1}{\Phi_h(z_1/L)}$, with $\Phi_h(z/L) = \left(1 - \frac{16z}{L}\right)^{-1/2}$.

The general solution for a confined PBL as obtained by Demuth [7] is

$$C_y = \frac{2Qqz_1^{\alpha}}{h^{\alpha+1}u_1} \times \left\{\gamma + \left(\frac{zR}{h}\right)^p \sum_{i=1}^{\infty} \frac{J_{\gamma-1}\left(\rho_{\gamma(i)}R^q\right) J_{\gamma-1}\left[\rho_{\gamma(i)}(z/h)^q\right]}{J^2_{\gamma-1}(\rho_{\gamma(i)})} \exp\left[-\frac{\rho^2_{\gamma(i)}q^2K_1x}{h^{\lambda}z_1^r u_1}\right]\right\}, \tag{25}$$

where $\lambda = \alpha + \beta - 2$, $\nu = (1-\beta)/\lambda$, $\gamma = (\alpha+1)/\lambda$, $r = \beta - \alpha$, $R = H_s/h$, $p = (1-\beta)/2$, $q = \lambda/2$, J_γ and $I_{-\nu}$ represent the Bessel function and modified Bessel function of first kind and order γ and $-\nu$, respectively, while $\rho_{\gamma(i)}$ are roots of J_γ.

3. – Models evaluation

The model performances have been evaluated against experimental ground-level concentration using tracer SF_6 data from the dispersion field campaign carried out in the Copenhagen area during atmospheric conditions going from moderately unstable to fully convective [19]. The tracer was released without buoyancy from a tower 115 m tall, and collected at the ground-level positions in up to three crosswind arcs of tracer sampling units. The sampling units were positioned at 2–6 km from the point of release. The site was mainly residential with a roughness length of 0.6 m. The meteorological conditions recorded during the dispersion experiments are summarised in table I where the convective velocity scale (w_*) is calculated from

$$w_* = u_*\left(\frac{h}{-\kappa L}\right)^{1/3}.$$

TABLE I. – *Summary of meteorological conditions during the experiments.*

Exp.	u_* (ms^{-1})	U (ms^{-1})		L (m)	w_* (ms^{-1})	h (m)
		10 m	115 m			
1	0.36	2.1	3.4	−37	1.8	1980
2	0.73	4.9	10.6	−292	1.8	1920
3	0.38	2.4	5.0	−71	1.3	1120
4	0.38	2.5	4.6	−133	0.7	390
5	0.45	3.1	6.7	−444	0.7	820
6	1.05	7.2	13.2	−432	2.0	1300
7	0.64	4.1	7.6	−104	2.2	1850
8	0.69	4.2	9.4	−56	2.2	810
9	0.75	5.1	10.5	−289	1.9	2090

TABLE II. – *Observed and modelled cross-wind integrated concentrations (normalized with emission) using the Copenhagen data set.*

Exp. No.	Distance (m)	Data (10^{-4} sm^{-2})	Model-GI (10^{-4} sm^{-2})	Model-GII (10^{-4} sm^{-2})	Model-KI (10^{-4} sm^{-2})	Model-KII (10^{-4} sm^{-2})
1	1900	6.48	7.15	6.67	4.35	6.32
	3700	2.31	4.12	3.70	2.20	4.10
2	2100	5.38	3.95	3.09	4.73	3.71
	4200	2.95	2.82	2.24	2.06	2.58
3	1900	8.20	8.25	6.35	7.28	7.53
	3700	6.22	5.62	4.41	3.45	5.40
	5400	4.30	4.25	3.18	2.32	4.35
4	4000	11.66	8.02	5.54	5.47	8.65
5	2100	6.72	7.05	5.19	15.02	6.14
	4200	5.84	5.77	4.46	5.41	5.63
	6100	4.97	4.75	3.57	3.51	4.78
6	2000	3.96	2.75	2.59	4.80	3.19
	4200	2.22	2.22	1.90	1.88	2.39
	5900	1.83	1.82	1.48	1.30	1.97
7	2000	6.70	4.75	4.04	3.61	4.10
	4100	3.25	3.17	2.56	1.67	2.62
	5300	2.23	2.60	2.03	1.29	2.22
8	1900	4.16	4.57	3.31	3.94	4.21
	3600	2.02	3.20	2.44	1.92	3.20
	5300	1.52	2.45	1.79	1.28	2.62
9	2100	4.58	3.65	3.08	4.31	3.60
	4200	3.11	2.50	2.16	1.92	2.44
	6000	2.59	1.90	1.60	1.31	1.93

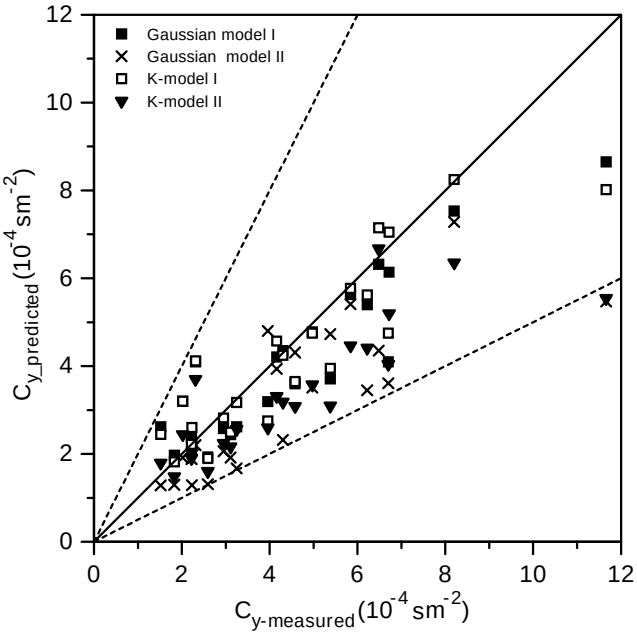

Fig. 1. – Scatter diagrams between the predicted and measured crosswind-integrated concentrations. Data between dashed lines are in factor of two.

Regarding the mean wind speed parameterisation, the KappaG model uses the power law functions proposed by Irwin [4], while the Gaussian model employs a constant value extrapolated from a log-law at source height.

In table II the observed and computed ground-level cross-wind concentrations for the four models (Gaussian model I and II and the K-model I and II) are presented.

Figure 1 shows the scatter diagram between observed and predicted integrated cross-wind concentrations of the four models. Analysis of results shows a good agreement between measurements and simulations for all models.

Table III presents the model performance evaluation statistics on Copenhagen data using the following statistical indices widely used in the model inter-comparison context (Hanna [20]):

$$\text{nmse (normalized mean square)} = \overline{(C_\mathrm{o} - C_\mathrm{p})^2}/\overline{C_\mathrm{o}C_\mathrm{p}} \ ,$$

$$\text{cor (correlation)} = \overline{(C_\mathrm{o} - \overline{C_\mathrm{o}})(C_\mathrm{p} - \overline{C_\mathrm{p}})}/\sigma_\mathrm{o}\sigma_\mathrm{p} \ ,$$

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

$$\text{fb (fractional bias)} = \left(\overline{C_\mathrm{o}} - \overline{C_\mathrm{p}}\right) / \left(0.5\left(\overline{C_\mathrm{o}} + \overline{C_\mathrm{p}}\right)\right) \ ,$$

where the subscripts o and p refer to observed and predicted quantities, and an overbar indicates an average.

The statistical evaluation highlights a quite satisfactory performance for all models: all the values for the numerical indices are within ranges that are characteristics of those found for other state-of-the-art models applied to other field datasets. In particular, the Gaussian model I and the K-model I show the better performances, nmse is equal to 0.07

TABLE III. – *Statistical indices evaluating the models performances.*

	nmse	fa2	cor	fb	fs
Gaussian model I	0.07	1	0.92	0.10	0.29
Gaussian model II	0.38	0.91	0.61	0.19	−0.19
K-model I	0.07	1	0.90	0.06	0.23
K-model II	0.21	0.96	0.84	0.29	0.48

and fa2 is 100%. This confirms that the approach for the dispersion parameterisations, which is the same for Gaussian and K models I, contains a realistic description of the eddies that contribute to the turbulent dispersion in the unstable boundary layer. For one typical Copenhagen tracer experiment, the computational time required for the Gaussian model I is about 1 s, while for the K-model I it is approximately 10 s.

An advantage of using the Gaussian model I is that the computer requirements are some orders of magnitude less than the K-model I. This is something fundamental when regulatory applications require climatological runs.

4. – Conclusions

Gaussian air pollution concentration is an exact solution of the advection-diffusion equation under a very restrictive hypothesis for PBL turbulence. Besides these limitations it has been widely used in regulatory air pollution applications because of their fast execution time. The spreading processes are usually expressed by semi-empirical sigmas obtained by fitting the asymptotic limits of Taylor's theory with experimental data. A recent approach proposed by [8-11] overcomes the necessity of such fitting by using directly the Hay and Pasquill [21] dispersion formula. The resulting dispersion parameterisations are just related to the scaling variables defining the turbulent state of PBL. Furthermore, this procedure allows to relate explicitly the spreading processes with the energy containing eddies and viscous dissipation.

A preliminary comparison study has been performed in this paper. Two Gaussian and two K-models have been compared utilising the Copenhagen dataset. The result of such comparison shows the good perfomances of the Gaussian model with sigmas calculated from Degrazia *et al.* [8] compared to a Gaussian model with sigmas from Weil and Brower [12]. On the other hand, the K-models comparison points out that the K-model I presents better results compared to K-model II. We conclude that both dispersion models that employ the turbulent parameterisation proposed by [8-11] provide the more realistic ground-level concentration field.

In the context of regulatory applications, when climatological runs are required, the Gaussian model I is preferable because it is the fastest despite the integral form of its sigmas.

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