A non-Gaussian puff model (*)

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Summary. — A model for the dispersion of passive non-Gaussian puffs is presented. The model is based on a general technique for solving the K-equation on the basis of the truncated Gram-Charlier expansion of the concentration field. The model performances are evaluated against experimental ground-level concentrations, using meteorological data collected near the ground.

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1. – Introduction

A distorting effect of the variation with height of the mean wind, both in speed and direction, is often evident in the development of puffs or plumes smoke. The effect is most evident in stable stratified conditions. In fact, windshear creates variance in the direction of the wind, vertical diffusion destroys this variance and tries to re-establish a non-skewed distribution. The interaction between vertical mixing and velocity shear is continuously effective.

In order to take into account the above phenomenon, we have developed a model for the dispersion of passive non-Gaussian puffs. The model is based on a general technique for solving the K-equation on the basis of the truncated Gram-Charlier expansion of the concentration field, and of the finite set of equations for the corresponding moments. In fact, the Gram-Charlier expansion of type-A is a classical method for approximating a given distribution having moments of any order and it consists, basically, of a truncated expansion in terms of Hermitian functions whose coefficients are chosen so as to reproduce the sequence of moments of the distribution up to a given order. In particular, the model is well suited to applications where we are

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interested mainly in some overall properties of the horizontal patterns, rather than in specific values at particular point receptors.

2. – The puff model

The advection diffusion equation describing the time evolution of the concentration C due to an instantaneous release at time $t = 0$ by an elevated source placed at (0, 0, 1), in a horizontally homogeneous atmospheric boundary layer is

$$(1)\quad \frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + dv\frac{\partial C}{\partial y} = \frac{\partial}{\partial z}K_z\frac{\partial}{\partial z}C + K_h\left(\frac{1}{d^2}\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right) + \delta(t)\,\delta(x)\,\delta(y)\,\delta(z-1),$$

where x is the along-wind coordinate, y the cross-wind one and z the height. δ means delta function, $(u, v, 0)$ is the wind velocity vector, K_z and K_h are the eddy diffusivities for vertical and horizontal turbulent transport, respectively. All variables are non-dimensional, the corresponding scale factors being given by H_s^2/K_s for time, $u_s H_s^2/K_s = d\cdot H_s$ for distance along the x-axis, H_s for the height and distance along the y-axis, K_s for diffusivities, u_s for wind speed and $Q/(d\cdot H_s^3)$ for concentration, where Q is the emission flux. K_s and u_s are meant to represent the values of the dimensional u and K profiles at the dimensional source H_s.

The initial condition is

$$\lim_{t\to 0^+} C(x, y, z, t) = 0$$

and the no-flux boundary conditions applied at the ground level and at the mixing layer height $z = z_i$ are

$$K_z\frac{\partial C}{\partial z} = 0 \qquad \text{for} \qquad z = 0 \ \text{ and } \ z = z_i\,.$$

Since C is exponentially small at asymptotic distances from the source on any horizontal plane, we can introduce the moments of its (x, y)-distribution:

$$(2)\qquad C_{m,n} = \int_{-\infty}^{\infty}\int x^m y^n C\,\mathrm{d}x\,\mathrm{d}y\,,$$

where m, n are non-negative integers.

Of course, $C_{m,n}$ are functions of height and of time.

If we multiply eq. (1) by $x^m y^n$ and if we integrate two times in x and y, after some calculations we obtain

$$(3)\qquad \begin{cases} \dfrac{\partial C_{0,0}}{\partial t} = DC_{0,0} + \delta(t)\,\delta(z-1)\,, \\ \dfrac{\partial C_{m,n}}{\partial t} = DC_{m,n} + muC_{m-1,n} + ndvC_{m,n-1} + \\ \qquad\qquad + K_h(1/d^2\, m(m-1)\,C_{m-2,n} + n(n-1)\,C_{m,n-2})\,, \end{cases}$$

for $m + n \neq 0$ and D the differential operator $(\partial/\partial z)\,K_z(\partial/\partial z)$.

That is, the time evolution of the moments of the concentration is governed by the double sequence of 1-dimensional diffusion equations, equivalent to the single three-dimensional (1).

The initial condition becomes

$$\lim_{t \to 0^+} C_{m,n} = 0$$

and the boundary conditions become

$$K_z \frac{\partial C_{m,n}}{\partial z} = 0 , \qquad \text{at } z = 0 \text{ and } z = z_i .$$

A classical method for approximating a given distribution having moments of any order is the Gram-Charlier expansion of type A, which consists, basically, of a truncated expansion in terms of Hermitian functions whose coefficients are chosen so as to reproduce the sequence of moments of the function up to a given order [1].

If Φ is a function approximated by the Gram-Charlier expansion truncated to the fourth order,

$$\Phi_i = \sum_{k=0}^{4} a_k M_k^i , \qquad i = 0, 1 \ldots 4 , \tag{4}$$

where M_k^i ($k = 0, 1, \ldots, 4$) are the moments of Φ_i (in our case the moments are evaluated from eq. (3)).

By direct use of the recurrence formulae satisfied by the Hermitian functions [2], it is possible to solve for the coefficients a_k [3].

If Φ is the one-variate function of the concentration $C(x)$ and S_k is the skewness and K_u is the kurtosis, we obtain [3]

$$C \cong C_0 \frac{e^{-\xi^2/2}}{\sigma\sqrt{2\pi}} \left[1 + \left(\frac{K_u - 3}{24} \right) (\xi^4 - 6\xi^2 + 3) + \frac{S_k}{6} \xi (\xi^2 - 3) \right], \tag{5}$$

where

$$\xi = \frac{x - b}{\sigma} ,$$

$$b = \frac{C_1}{C_0} ,$$

$$\sigma^2 = \frac{C_2}{C_0} - b^2 ,$$

$$S_k = \frac{1}{\sigma^3} \left[\frac{C_3}{C_0} - 3b\sigma^2 - b^3 \right],$$

$$K_u = \frac{1}{\sigma^4} \left[\frac{C_4}{C_0} - 6b^2\sigma^2 - 4b\sigma^3 S_k - b^4 \right].$$

3. – Boundary layer parameterization

In order to evaluate the diffusion coefficients that are in eqs. (3), we have used the boundary layer parameterization proposed by Pleim and Chang [4].

Following Pleim and Chang [4], during stable and near-neutral conditions ($H/L \geqslant -10$), we adopted

$$K_z = \frac{k u_* z (1 - z/z_i)^2}{\Phi_h(z/L)} \,. \tag{6}$$

During convective conditions ($H/L < -10$) the friction velocity (u_*) was replaced by the convective velocity (w_*) as scaling velocity to give [4]

$$K_z = k w_* z (1 - z/z_i) \,, \tag{7}$$

where the convective velocity is defined as follows:

$$w_* = (g/\theta_0 \overline{w' \theta'_0} \, z_i)^{1/3} \,, \tag{8}$$

where g is the gravitational acceleration, w is the vertical velocity, θ the potential temperature and $\overline{w' \theta'_0}$ is the surface kinematics heat flux. The prime "$'$" means turbulent fluctuations variables.

For the horizontal eddy diffusivity in unstable conditions we use [5]

$$K_h = 0.1 w_* z_i \,. \tag{9}$$

In neutral-stable conditions [6]

$$K_h = 2 K_{Mz} \tag{10}$$

where K_{Mz} is the maximum of K_z.

The parameterization adopted is based on fundamental parameters of atmospheric boundary layer: that is, it is possible to evaluate them if L and u_* are known. In recent years, with the works of Holtslag and Van Ulden [7], Weil and Brower [8], Van Ulden and Holtslag [9], Trombetti *et al.* [10] and Hanna and Paine [11] it turns out that the fundamental parameters of atmospheric boundary layer (L and u_*) can be evaluated by measurements at ground level. Moreover, Beljaars and Holtslag [12] presented a software library for the calculation of the parameters of atmospheric boundary layer from a single wind speed and air temperature, aerodynamic roughness length and cloud cover from SYNOP observations.

For the above considerations, the model presented can be applied routinely using as input simple ground-level meteorological data acquired by an automatic network.

4. – Preliminary validation *vs.* experimental data

We have evaluated the performances of the puff model using the Copenhagen data set [13]. The Copenhagen data set is composed of tracer SF_6 data from dispersion experiments carried out in the northern part of Copenhagen. 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

TABLE I. – *Meteorological data used (from Gryning* [15] *and Gryning et al.* [14]).

Run	u (m/s)	u_* (m/s)	L (m)	w_* (m/s)	H (m)	H/L
1	3.4	0.37	−46	1.7	1980	−43
2	10.6	0.74	−384		1920	−5
3	5.0	0.39	−108		1120	−10
4	4.6	0.39	−173		390	−2.3
5	6.7	0.46	−577		820	−1.4
6	13.2	1.07	−569		1300	−2.3
7	7.6	0.65	−136	2.1	1850	−1.4
8	9.4	0.70	−72	2.1	810	−11
9	10.5	0.77	−382		2090	−5.5

were positioned 2–6 km from the point of release. We have used the values of the crosswind-integrated concentrations normalised with the tracer release rate from Gryning *et al.* [14]. Tracer releases typically started 1 hour before the start of tracer sampling and stopped at the end of the sampling period; the average sampling time was 1 hour. The site was mainly residential with a roughness length of 0.6 m.

Table I shows the meteorological data [14, 15] utilised for the validation of the

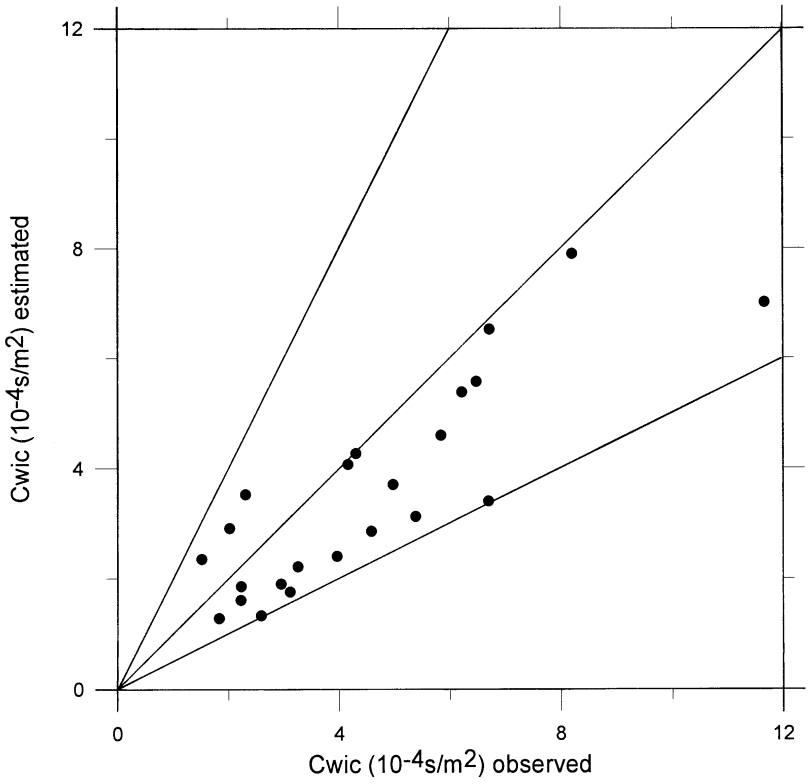

Fig. 1. – Comparison between predicted and observed crosswind-integrated concentrations C_{wic} normalized by the emission rate Q times 10^4. Data between dotted lines are within a factor of two.

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

Model	nmse	r	fa2	fb	fs
Presented model	0.16	0.85	1.00	0.23	0.26
VHDM	0.13	0.78	0.96	0.06	0.52
HPDM	0.16	0.78	1.00	0.16	0.39
IFDM	0.16	0.68	0.96	0.01	0.21
UNPUFF	0.46	0.36	0.70	0.28	0.28
OML	0.52	0.89	0.56	0.57	0.58
UK-ADMS	0.86	0.91	0.35	0.74	0.73

model. In fig. 1 the measured ground-level concentration values are presented against the computed ones.

Moreover, table II presents some statistical indices defined as normalised mean-square error (nmse), correlation coefficient (r), factor of two (fa2), fractional bias (fb) and fractional standard deviation (fd),

$$\text{nmse} = \frac{\overline{(C_\text{o} - C_\text{p})^2}}{\overline{C}_\text{o}\overline{C}_\text{p}} ,$$

$$r = \frac{\overline{(C_\text{o} - \overline{C}_\text{o})(C_\text{p} - \overline{C}_\text{p})}}{\sigma_\text{o}\sigma_\text{p}} ,$$

$$\text{fa2} = \text{data for which } 0.5 \leqslant C_\text{p}/C_\text{o} \leqslant 2 ,$$

$$\text{fb} = 2\,\frac{\overline{C}_\text{o} - \overline{C}_\text{p}}{\overline{C}_\text{o} + \overline{C}_\text{p}} ,$$

$$\text{fd} = 2\,\frac{\sigma_\text{o} - \sigma_\text{p}}{\sigma_\text{o} + \sigma_\text{p}} ,$$

where the subscripts “o” and “p” are for the observed and predicted concentrations, respectively, while σ is the standard deviation.

Moreover, to compare the performance of the non-Gaussian puff model with that of other models, table II reports the results obtained on the same data sets using the VHDM model [16] and the models that participated in the model validation exercise during the *Workshop on Operational Short-range Atmospheric Dispersion Models for Environmental Impact Assessment in Europe* [17]: HPDM [18], IFDM [19], INPUFF [20], OML [21], UK-ADMS [22].

Statistical indices show that all models tend to underestimate the air pollution concentrations measured during the Copenhagen experiment and confirm the reliability of our model results.

5. – Conclusions

A non-Gaussian puff model has been presented. The model can be applied routinely using as input simple ground-level meteorological data acquired by an automatic network. In fact it uses diffusion parameterizations based on the similarity theory and, in recent years, it turns out that the fundamental parameters for describing the characteristics of the atmospheric surface and boundary layer can be evaluated by measurements at the ground. Preliminary model performances evaluation confirm the reliability of the model results.

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