IL NUOVO CIMENTO Vol. 25 C, N. 3 Maggio-Giugno 2002

Two-dimensional dispersion analytical approach: Eddy diffusivities depending on source distance(*)

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(ricevuto il 9 Novembre 2000; revisionato il 5 Novembre 2001; approvato il 5 Dicembre 2001)

Summary. — An analytical air quality dispersion approach based on the steady-state two-dimensional advection-diffusion equation is presented. The solution employs a spectral method and is analytical in the sense that no approximation is made along its derivation. The approach is valid for homogeneous turbulence and for situations of uniform mean wind speed, and for practical purposes, to elevated releases that occur in neutral stability conditions without strong buoyancy. To simulate and compare the results of this approach against observed ground-level crosswind-integrated concentration two eddy diffusivities are considered. The first eddy diffusivity depends on the distance from the source while the second one assumes a constant value independent of the source distance. It is found that the memory effect contained in the eddy diffusivity, which is a function of downwind distance from the source, allows a better description of the turbulent dispersion of atmospheric contaminants released by an elevated continuous point source.

PACS 92.60.Sz – Air quality and air pollution.
PACS 92.60.Fm – Boundary layer structure and processes.

1. – Introduction

The Eulerian dispersion model concept has been largely applied for estimating ground-level concentrations, due to low and high stack emission, and is usually suitable for regulatory use in air quality models. In principle, from the advection-diffusion equation it is possible to obtain a practical model of dispersion from a continuous point source, given appropriate boundary and initial conditions, and a knowledge of the time and space fields of U (mean wind speed) and K_α (eddy diffusivities, with $\alpha = x, y, z$).

Much of the research on turbulent dispersion has been related to the specification of turbulent concentration fluxes in order to allow for the solution of the Reynolds averaged

(*) The authors of this paper have agreed to not receive the proofs for correction.

advection-diffusion equation. The process for specifying the turbulent fluxes parameterization is called the turbulent transport closure problem. The most common scheme for closing the equation is to relate turbulent concentration fluxes to the gradient of the mean concentration by eddy diffusivities which are functions of not only turbulence (*e.g.*, energy-containing eddy length and characteristic velocity scales), but also of distance from the continuous point source. Although the application of the eddy diffusivity concept depends on the geometry of the source distribution, it has been found useful in many practical applications [1, 2].

An extensive number of works concerning analytical and numerical solutions of the advection-diffusion equation for non-constant eddy diffusivities (eddy diffusivities that are functions of height z) that do not depend on the distance from the source is available in the literature. Among them we cite the works by Huang [3], Demuth [4], Nieuwstadt [5], Yeh and Huang [6], and Tirabassi [7].

On the other hand, literature regarding solutions of the advection-diffusion equation with eddy diffusivities that are functions of downwind distance is scarce [2].

In this paper, our attention is focused upon the determination of an analytical solution for the steady-state two-dimensional advection-diffusion equation. To determine this solution the General Integral Transform Technique (GITT) is used, *i.e.* the averaged crosswind concentration for the y variable is expanded in a truncated series functions of the eigenfunctions of constructed Sturm-Liouville problem for the z variable. Replacing this presumption in the advection-diffusion equation and using the orthogonality property of the eigenfunction, a set of first-order ordinary differential equations are obtained, whose solution is well known. A vast literature concerning the application of GITT to solve multidimensional heat transfer and fluid mechanic problems is available that it is impossible to mention all of them. Just for illustration is cited the recent book written by Cotta and Mikhailov [8].

In the present study, eddy diffusivities that are functions of distance from the source in homogeneous turbulence are considered. These eddy diffusivities contain the characteristic velocity and length scales (w_* and unstable PBL height) of energy-containing eddies and can describe dispersion in the near and intermediate fields of an elevated source, *i.e.* when the scale of the plume is smaller than the scale of the turbulence.

To our knowledge, the application of the reported method to the analytical solution of the advection-diffusion equation with the eddy diffusivity depending on the source distance to calculate the ground-level crosswind-integrated concentration and hence investigate the influence of the retention of the memory effect in the turbulent dispersion process of contaminants released by an elevated continuous point source, is the novelty of this work. Simulations and comparisons against measured ground-level crosswind-integrated concentration [9, 10] are reported.

2. – Analytical approach

The study of transport and dispersion of pollutants in the atmosphere is mostly described by the advection-diffusion equation, obtained by parameterizing the concentration turbulent fluxes in the continuity equation employing the gradient transport model or K-theory. For a Cartesian coordinate system in which the x direction coincides with that of the average wind, the steady-state diffusion equation is written as Arya [2]

$$U\frac{\partial \overline{c}}{\partial x} = \frac{\partial}{\partial x}\left(K_x\frac{\partial \overline{c}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial \overline{c}}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial \overline{c}}{\partial z}\right) , \tag{1}$$

where $\overline{c}$ denotes the average concentration, U is the mean wind speed in the x direction and K_x, K_y and K_z are the eddy diffusivities in the x, y and z directions, respectively [11, 12]. Neglecting the longitudinal diffusion with respect to wind advection ($U \gg u'$), since it is assumed that the advection mean speed is dominant over the turbulent transport in the longitudinal and the turbulent diffusion in the wind direction is neglected compared to the advection (slender plume approximation). These approximations are valid when the scale of the turbulent transport is smaller than the plume dimensions [11, 12] and considering a vertical eddy diffusivity ($K_z(x)$) described by a large-eddy length and a velocity scale, and depending on the downwind source distance, x, the crosswind integration of eq. (1) leads to

$$U\frac{\partial\overline{c_y}(x,z)}{\partial x} = K_z(x)\frac{\partial^2\overline{c_y}(x,z)}{\partial z^2}\,, \qquad \overline{c_y}(x,z)\,,\ \ 0<z<z_i;\ \ 0<x<\infty\,, \tag{2}$$

where $\overline{c_y}(x,z)$ represents the average crosswind-integrated concentration and z_i the unstable PBL height. Subject to the boundary conditions of zero flux at the ground and PBL top, and a source with emission rate Q at height H_s, that respectively are

$$K_z(x)\frac{\partial\overline{c_y}(x,z)}{\partial z} = 0\,, \qquad em\ z = 0, z_i\ , \tag{3}$$

$$U\ \overline{c_y}(0,z) = Q\delta(z-H_s)\ . \tag{4}$$

Here δ is the generalized delta-function. The fact that $K_z(x)$ for all heights will be identical (it is not a function of z) limits this approach (2) to situations where the turbulence is homogeneous, and, as a consequence, restricts their application to much fewer atmospheric conditions and locations.

Following the idea of the spectral method [8], the solution of problem (2) is assumed to be written as

$$\overline{c_y}(x,z) = \sum_{n=0}^{\infty} A_n(x)\ Z_n(z)\ . \tag{5}$$

Observe that in the z direction it is possible to construct the ensuing Sturm-Liouville problem

$$\frac{\mathrm{d}^2\,Z(z,\beta_n)}{\mathrm{d}z^2} + \beta_n^2\,Z(z,\beta_n) \,=\, 0\,, \qquad \forall n\in\mathbb{N}, \tag{6}$$

$$\frac{\mathrm{d}\,Z(z,\beta_n)}{\mathrm{d}z} \,=\, 0\,, \qquad em\ z \,=\, 0\ , \tag{7}$$

$$\frac{\mathrm{d}\,Z(z,\beta_n)}{\mathrm{d}z} \,=\, 0\,, \qquad em\ z \,=\, z_i\ , \tag{8}$$

that has a well-known solution. Here, the eigenvalues β_n and the eigenfunctions $Z(z,\beta_n)$ are taken from Özisik [13], table (2.4). Subsequently in order to determine the unknown function $An(x)$, we replace (5) in eq. (2). Following this procedure, and bearing in mind that the set of eigenfunctions $Z_n(z)$ constitutes a set of linearly independent functions, we readily obtain

$$U\frac{\mathrm{d}\,A_n}{\mathrm{d}x} = -\beta_n^2\,K_z(x)\,A_n(x)\,, \qquad \forall\, n \in \mathbb{N}\,, \tag{9}$$

where $\mathbb{N}$ denotes the set of natural numbers. The solution for eq. (9) is well established [14] and has the form

$$A_n = a_n \exp\left[\frac{-\beta_n^2}{U}\int K_z(x)\,\mathrm{d}x\right]\,, \qquad \forall\, n \in \mathbb{N}\,. \tag{10}$$

To this point, it is important to realize that our assumption for the solution of problem (2) is correct because the functions A_n are uniquely determined, except for the arbitrary constant a_n, which depend on the boundary conditions. Indeed replacing eq. (10) into eq. (5), the solution of problem (2) is recast as

$$\overline{c_y}(x,z) = \sum_{n=0}^{\infty} a_n\, Z_n(z,\beta_n)\exp\left[\frac{-\beta_n^2}{U}\int K_z(x)\,\mathrm{d}x\right]\,. \tag{11}$$

Finally applying the boundary condition (4) and taking advantage of the orthogonality property of the eigenfunctions $Z_n(z,\beta_n)$, we attain the arbitrary coefficients a_n and consequently, the following solution for the problem (2):

$$\overline{c_y}(x,z) = \frac{Q}{U z_i} + \frac{2Q}{U z_i}\sum_{n=1}^{N}\cos(\beta_n\,H_s)\,\cos(\beta_n\,z)\exp\left[-\frac{\beta_n^2}{U}\int_0^x K_z(\varsigma)\,\mathrm{d}\varsigma\right]\,. \tag{12}$$

The analytical solution (12) for the crosswind-integrated pollutant concentration downwind from an elevated, non-buoyant point source can be used under only very limited circumstances: neutral stability, homogeneous and Gaussian turbulence, when buoyance effect is negligible. The vertical component of the eddy diffusivity is not height dependent in this approach, limiting the applicability. However, for the subset of problems for which the approach is applicable, the novel description for vertically independent K_z making it a function of downwind distance x, has extended the ability of this dispersion approach to more accurately represent downwind pollutant concentrations when compared against field data. Equation (12) is analytical in the sense that no approximation is made along its derivation.

The following vertical eddy diffusivity $K_z(x)$ depending on the source distance used in eq. (12) is based on spectral properties and Taylor's statistical diffusion theory, and, has been derived by Degrazia [15] for an unstable PBL:

$$\frac{K_z(x)}{w_*\,z_i} = 0.054\,\psi^{1/3}\int_0^{\infty}\frac{\sin[4.71\,\psi^{1/3}\,X\,n']}{n'\,(1+n')^{5/3}}\mathrm{d}n'\,, \tag{13}$$

where w_* is the convective velocity scale, $\psi = (\varepsilon z_i)/{w_*}^3$ is the non-dimensional molecular dissipation rate function (ε is the dissipation rate of turbulent kinetic energy), and $X = (x\,w_*)/(U\,z_i)$ can be thought of as a non-dimensional time since it is the ratio of travel time x/U to the convective timescale z_i/w_*, and n' is a dimensionless frequency.

The $K_z/w_* z_i$ as given by eq. (13) is initially zero, increases with X at first linearly and then more slowly, and finally tends to a constant value. This constant value, appropriate for far-source dispersion, is equal to

$$\frac{K_z}{w_* z_i} = 0.085 \, \psi^{1/3} \, . \tag{14}$$

The eddy diffusivity (13), as a function of downwind distance, yields a description of diffusion in the near, intermediate, and far fields of an elevated source. A detailed derivation of (13) and (14) can be found in the appendix. Thus, in this study we consider the vertical eddy diffusivities (13) and (14) for an elevated continuous source in an unstable PBL. By elevated, we mean heights are above 100 m in unstable conditions. At these heights we suppose that K_z is only weakly dependent on the turbulence properties (it is not a function of z), with the dimension and velocity of the energy-containing eddies being respectively proportional to the inversion height z_i and velocity w_*.

3. – Approach evaluation

The performance of the present approach (eqs. (12), (13), and (14)) has been evaluated against experimental ground-level concentrations using tracer SF6 data from dispersion experiments carried out in the northern part of Copenhagen, described in Gryning *et al.* [9]. The tracer was released without buoyancy from a tower at a height of 115 m, and collected at the ground-level positions at a maximum of 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 [16] and Gryning *et al.* [9] utilized for the validation of the proposed approach. The meteorological data used was collected near the ground, so the comparison can be said to simulate the values given by a routine use of the approach. The Copenhagen dataset was chosen since most of the experiments were performed under the neutral stability conditions, and without strong buoyancy, so that ground-level crosswind-integrated concentration can be simulated by an advection-diffusion equation.

TABLE I. – *Summary of meteorological conditions during the experiments of Copenhagen* [9].

Exp No.	U ($\mathrm{ms^{-1}}$)	u^* ($\mathrm{ms^{-1}}$)	L (m)	w^* ($\mathrm{ms^{-1}}$)	z_i (m)	H_s/z_i	z_i/L
1	3.40	0.37	−46	1.76	1980	0.058	−43
2	10.60	0.74	−384	1.72	1920	0.060	−5
3	5.00	0.39	−108	1.15	1120	0.103	−10
4	4.60	0.39	−173	0.69	390	0.295	−2.3
5	6.70	0.46	−577	0.70	820	0.140	−1.42
6	13.20	1.07	−569	1.91	1300	0.088	−2.3
7	7.60	0.65	−136	2.11	1850	0.062	−14
8	9.40	0.70	−72	2.13	810	0.142	−11
9	10.50	0.77	−382	1.84	2090	0.055	−5.5

The stability parameter z_i/L, where L is the Monin-Obukhov length, indicates cases where the unstable PBL presents weak to moderate convection. Both eqs. (12) and (14) contain the unknown function ψ. This mean dissipation of turbulent kinetic energy is important to quantify dispersion parameters since the order of magnitude of the mean dissipation of turbulent kinetic energy per unit time per unit mass of fluid, ε, is determined only by those quantities which characterize the large eddies.

Therefore, for elevated releases in an unstable PBL, ε is described in terms of w_* and z_i which are velocity and length scales of the energy-containing eddies, respectively. Observations and numerical simulations in central regions of the unstable PBL show that $\psi \simeq 0.4$ [17-19]. Nevertheless, several field experiments in unstable PBL [20-23] emphasize that for dimensionless heights in the range $0.05 < z/zi < 0.3$ the values of ψ are much greater than 0.4. According to Druilhet *et al.* [22], ψ profile can be approximated by the exponential law

$$\psi = 1.26 \exp\left[-\frac{z}{0.8\, z_i}\right], \qquad 0 < -z/z_i < 0.8\,. \tag{15}$$

On the other hand, based on the Minnesota and Aschurch experiments [19], the dissipation function ψ can be described as follows [24]:

$$\psi = 1.5 \,-\, 1.2(z/z_i)^{1/3}\,. \tag{16}$$

Finally, Guillemet *et al.* [23] suggest the following fitting curve for the dissipation rate of turbulent kinetic energy:

$$\psi = [0.55 \,+ 0.05(z/z_i)^{-2/3}]^{3/2}\,, \qquad 0.03 < z/z_i < 0.3\,. \tag{17}$$

Considering the dimensionless source heights (H_s/z_i) of Copenhagen (table I), it is possible to select for H_s/z_i an average value equal to 0.11. Now, calculating ψ from eqs. (15), (16) and (17) in the dimensionless average source height $H_s/z_i = 0.11$, yields an average value for $\psi^{1/3}$ equal to 0.97.

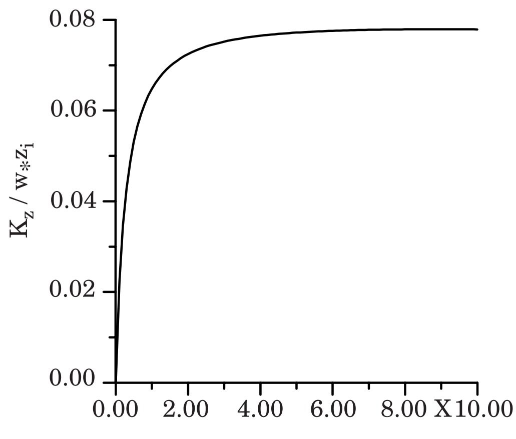

Fig. 1. – Eddy diffusivity ($K_z/w_*\, z_i$) from eq. (13), as a function of the non-dimensional distance $X = x\, w_* \,/\, u\, z_i$.

TABLE II. – *Observed and modeled ground-level crosswind-integrated concentrations* $\overline{c_y}(x,0)/Q$ *at different distances from the source of Copenhagen experiments.*

Exp. No.	Distance (km)	$X = \frac{xw_*}{Uz_i}$	Data ($\times 10^{-4}$sm^{-2})	Model (eqs. (12), (13)) ($\times 10^{-4}$sm^{-2})	Model (eqs. (12), (14)) ($\times 10^{-4}$sm^{-2})	Gaussian model ($\times 10^{-4}$sm^{-2})
1	1.9	0.496	6.48	6.29	4.06	6.32
	3.7	0.967	2.31	4.014	2.94	4.10
2	2.1	0.177	5.38	3.74	2.16	3.71
	4.2	0.355	2.95	2.60	1.57	2.58
3	1.9	0.39	8.20	7.56	5.18	7.53
	3.7	0.76	6.22	5.54	3.86	5.40
	5.4	1.11	4.30	4.26	3.24	4.35
4	4.0	1.54	11.66	8.53	7.47	8.65
5	2.1	0.27	6.71	5.85	5.53	6.14
	4.2	0.53	5.84	5.83	4.38	5.63
	6.1	0.78	4.97	4.98	3.76	4.78
6	2.0	0.22	3.96	3.18	2.18	3.19
	4.2	0.47	2.22	2.38	1.59	2.39
	5.9	0.66	1.83	1.95	1.36	1.97
7	2.0	0.3	6.70	4.12	2.45	4.10
	4.1	0.62	3.25	2.59	1.75	2.62
	5.3	0.79	2.23	2.18	1.55	2.22
8	1.9	0.53	4.16	4.19	3.16	4.21
	3.6	1.01	2.02	3.14	2.42	3.20
	5.3	1.48	1.52	2.54	2.04	2.62
9	2.1	0.18	4.58	3.64	2.03	3.60
	4.2	0.35	3.11	2.45	1.47	2.44
	6.0	0.52	2.59	1.92	1.22	1.93

The behaviour of the vertical eddy diffusivity, as given by eq. (13), is presented in fig. 1. We can observe from this figure, and from table II, that for various distances X involved in the Copenhagen experiment, the K_z asymptotic value (eq. (14)) is not reached. As a consequence, eq. (13) represents a formula appropriate to describe dispersion in the near and intermediate fields of an elevated source.

As a test for the approach (12), and also to analyse the influence of the memory effect in the turbulent transport, the parameterization (13), and their asymptotic limit eq. (14), with $\psi^{1/3} = 0.97$, are used to simulate the ground-level crosswind-integrated concentrations $\overline{c_y}(0,z)$ of Copenhagen. In table II the measured and computed ground-level crosswind-integrated concentrations of the present approach and the Gaussian model of Degrazia [10] are presented.

Figure 2 shows the observed and predicted scatter diagram of ground-level crosswind-integrated concentrations using the approach (12) with eddy diffusivities given by eq. (13) and eq. (14) and the results of Degrazia [10]. In this respect it is important to note that a better fitting was encountered for the values of eddy diffusivity $K_z(x)$ evaluated by

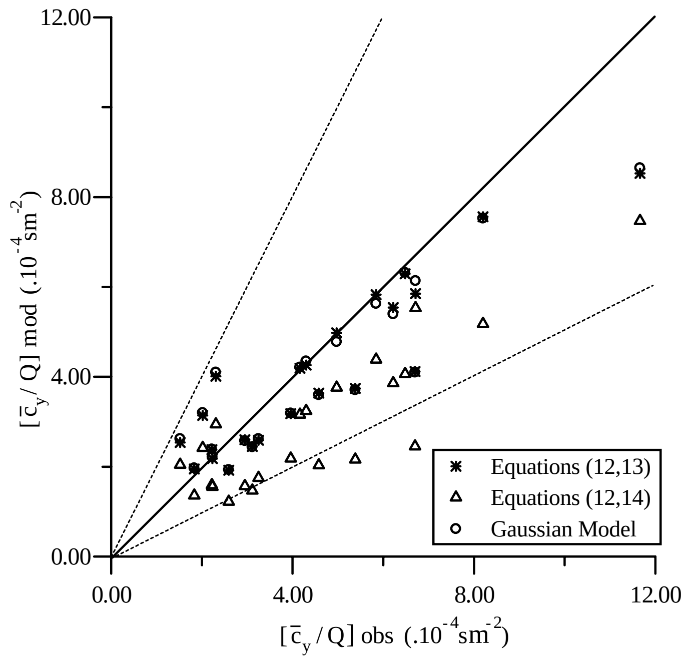

Fig. 2. – Observed $[\overline{c_y}/Q]_{\mathrm{obs}}$ and predicted $[\overline{c_y}/Q]_{\mathrm{mod}}$ crosswind ground-level–integrated concentration, normalized with emission $Q\,(\times 10^{-4a}\mathrm{sm}^{-2})$, scatter diagram for the solution of eqs. (12), (13), (12), (14) and Gaussian model.

eq. (13) (K_z varying with the source distance) and for the Gaussian model.

Subsequently, the datasets were applied to the following statistical indices [25], where subscripts "o" and "p" refer to observed and predicted quantities, and an overbar indicates an average:

$$\text{Nmse (normalized mean square error)} = \frac{\overline{(c_{\mathrm{o}} - c_{\mathrm{p}})^2}}{\overline{c_{\mathrm{o}}}\,\overline{c_{\mathrm{p}}}}.$$

$$\text{Cor (correlation)} = \frac{\overline{(c_{\mathrm{o}} - \overline{c_{\mathrm{o}}})(c_p - \overline{c_{\mathrm{p}}})}}{\sigma_{\mathrm{o}}\,\sigma_{\mathrm{p}}}.$$

$$\text{Fb (fractional bias)} = \frac{\overline{c_{\mathrm{o}}} - \overline{c_{\mathrm{p}}}}{0.5(\overline{c_{\mathrm{o}}} + \overline{c_{\mathrm{p}}})}.$$

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

	Nmse	Cor	Fb	Fs	Fa2
$c_y(x,0)$ - eqs. (12), (13)	0.07	0.917	0.099	0.292	1.00
$c_y(x,0)$ - eqs. (12), (14)	0.31	0.872	0.420	0.428	0.783
Gaussian M. [10]	0.08	0.870	0.100	0.310	1.00
$c_y(x,0)$ Gryning *et al.* [9]	0.00	1.00	0.00	0.00	1.00

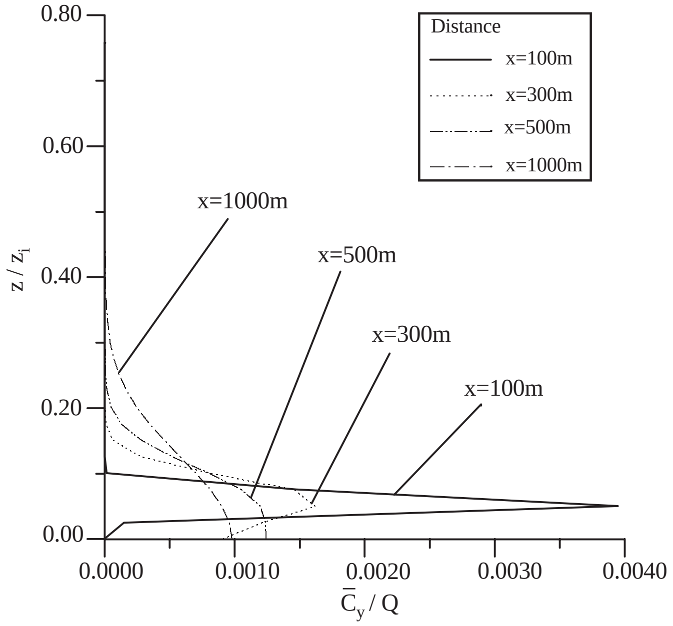

Fig. 3. – Vertical concentration profile of crosswind-integrated concentration, normalized with emission ($\overline{c_y}/Q$), as a function of z/z_i, for different distances X (experiment 1, table I).

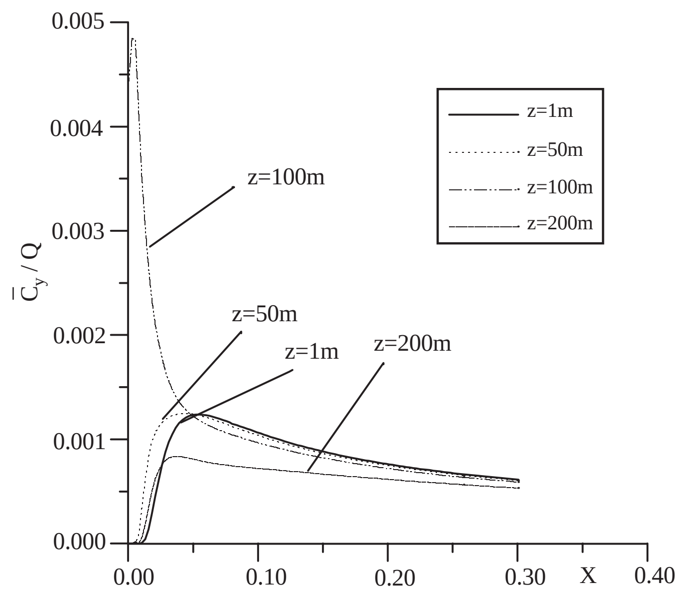

Fig. 4. – Distribution of crosswind-integrated concentration $\overline{c_y}/Q$, normalized with emission Q, for different heights z/z_i, as a function of X ($X = x\,w_*\,/\,u\,z_i$) (experiment 1, table I).

$$\text{Fs (fractional standard deviation)} = 2\frac{\sigma_{\text{o}} - \sigma_{\text{p}}}{\sigma_{\text{o}} + \sigma_{\text{p}}}.$$

Fa2 = fraction of c_{o} values within a factor of 2 of corresponding c_{p} values.

These results are compared with those obtained from Gryning *et al.* [9] and the Gaussian result [10], and are shown in table III.

A very good agreement with the Gryning results was obtained with the proposed approach that considers the K_z value to vary with the distance from source (eq. (13)).

By analysing the sensitivity of the present approach (eqs. (12) and (13)), and by using data from Copenhagen Experiment 1, we show in figs. 3 and 4, respectively, the plots of crosswind-integrated concentration, normalized with emission ($\overline{c_y}/Q$) as a function of z/z_i (for different distances) and crosswind-integrated concentration, normalized with emission ($\overline{c_y}/Q$) as a function of X (for different heights). These plots confirm that the approach exhibits a Gaussian behavior simulating a uniform concentration field for large distances X.

4. – Conclusions

This paper describes the development and testing of an analytical approach that simulates dispersion of contaminants into a PBL. The approach is based on the advection-diffusion equation and is solved by spectral method. It is important to notice that the solution encountered is analytical since no approximation is made along its derivation. Therefore, due to the analytical feature of this solution, it is possible to improve the coincidence of significant digits by increasing the number of summed terms in the solution. All the calculations were runned in a microcomputer with negligible computational effort and the results attained have an accuracy of ten significant digits.

The proposed approach considers a vertical eddy diffusivity varying with distance from the source in homogeneous turbulence with uniform mean wind speed everywhere and was validated with the data of Copenhagen experiments [16] and compared with Gryning numerical results [9] and with Degrazia Gaussian results [10].

To investigate the memory effect, which is consistent with the prediction of the Taylor statistical diffusion theory and, therefore, reinforce our confidence in the approach, a numerical comparison is also made with the results that come out of a simulation using the asymptotic constant vertical eddy diffusivity (eq. (14)) valid for large diffusion time.

The statistical analysis of the results shows a good agreement between the results of the proposed approach with with the experimental ones, Gaussian and Gryning results. Furthermore, it is important to emphasize that the results obtained with the eddy diffusivity depending on the source distance (eq. (13)) are better than the ones reached with asymptotic constant eddy diffusivity (eq. (14)), valid only for the far field of an elevated source. This result suggests that the inclusion of the memory effect, as modelled by Taylors theory, improves the description of the turbulent transport process of atmospheric effluent released by an elevated continuous point source.

These improved results, depicted in table III (Nmse, Cor, Fb, Fs, Fa2), are a consequence of a vertical eddy diffusivity described in terms of energy-containing eddies and this is a function of the downwind distance from the source.

Finally, we would like to point out that this analytical approach (12) for the crosswind-integrated pollutant concentration downwind from an elevated, non-buoyant point source can be used under only very limited circumstances: neutral stability, homogeneous and Gaussian turbulence, when buoyance effect is negligible. The vertical component of the eddy diffusivity is not height dependent in this approach, limiting the applicability. However, for the subset of problems for wich the approach is applicable, the novel description for vertically independent K_z making it a function of downwind distance x, has extended the ability of this dispersion approach to more accurately represent downwind pollutant concentrations when compared against field data. To handle more realistic problems, our future work is focused in the application of this formalism to solve the advection-diffusion equation, now considering the height and source dependence of the eddy diffusivity and the height variation of wind speed. To reach this goal, the height is discretized onto intervals such that in each interval we assume average values for the eddy diffusivity and wind speed. The global solution is then constructed considering continuity of the contaminant concentration and flux concentration at the interfaces.

* * *

This work was produced and supported under the auspices of the CAPES.

Appendix A.

Derivation of eqs. (9) and (10)

To obtain downwind distance-dependent K_α, we start with the formula for the dispersion parameter σ_α as given by Pasquill and Smith [11, 26]:

$$\sigma_\alpha^2 = \frac{\sigma_i^2\,\beta_i^2}{\pi^2}\int_0^\infty F_i^{\mathrm{E}}(n)\left[\frac{\sin^2(n\pi t\,/\,\beta_i)}{n^2}\right]\mathrm{d}n\,, \tag{A.1}$$

with $\alpha = x, y, z$; $i = u, v, w$, where $F_i^{\mathrm{E}}(n)$ is the value of the Eulerian spectrum of energy normalized by the Eulerian velocity variance σ_i^2, and β_i is defined as the ratio of the Lagrangian to the Eulerian integral time scales, n is the frequency and t is the travel time. An expression for the time-dependent eddy diffusivity was derived by Batchelor [27]:

$$K_\alpha = \frac{1}{2}\frac{\mathrm{d}\sigma_\alpha^2}{\mathrm{d}t}\,, \tag{A.2}$$

so that from eqs. (A.1) and (A.2) we obtain

$$K_\alpha = \frac{\sigma_i^2\,\beta_i}{\pi}\int_0^\infty F_i^{\mathrm{E}}(n)\frac{\sin(2n\pi t\,/\,\beta_i)}{n}\mathrm{d}n\,. \tag{A.3}$$

The equation for Eulerian velocity spectra under unstable conditions can be expressed as follows [28]:

$$\frac{n\,S_i^{\mathrm{E}}(n)}{w_*^2} = \frac{1.06\,c_i\,(f/q)(\psi/q)^{2/3}(z/z_i)^{2/3}}{(fm)_i^{5/3}[1+(1.5/(fm)_i)(f/q)]^{5/3}}\,, \tag{A.4}$$

where $c_i = \alpha_i\alpha_u(2\pi\kappa)^{-2/3}$, $\alpha_u = 0.5 \pm 0.05$ and $\alpha_i = 1, 4/3, 4/3$ for u, v and w components, respectively [29]; $\kappa = 0.4$ is the Von Karmann constant, $f = (nz)/U$ is the non-dimensional frequency, z is the height above the ground, U is the mean wind speed,

$(fm)_i$ is the normalized frequency of the spectral peak in the neutral stratification, $q = (fm^*)_i\,(fm)_i^{-1}$ is a stability function, where $(fm^*)_i$ is the normalized frequency of the spectral peak regardless of stratification; z_i is the unstable boundary layer height; w_* is the convective velocity scale and, finally, the non-dimensional molecular dissipation rate function is given by

$$\psi = \frac{\varepsilon\, z_i}{w_*}\,. \tag{A.5}$$

The above α_i values derive from the turbulence isotropy in the inertial subrange. Integrating $S_i^{\mathrm{E}}(n)$ in (A.1) over all frequencies range, one obtains the following Eulerian velocity variance:

$$\sigma_i^2 = \frac{1.06}{(fm)_i^{5/3}}\left(\frac{\psi}{q}\right)^{2/3}\frac{z\,w_*^2}{U\,q}\int_0^\infty\left[1+\frac{1.5}{(fm)_i}\frac{n\,z}{U\,q}\right]^{-5/3}\mathrm{d}n\,, \tag{A.6}$$

and finally

$$\sigma_i^2 = \frac{1.06\,c_i}{(fm)_i^{2/3}}\left(\frac{\psi}{q}\right)^{2/3}\left(\frac{z}{z_i}\right)^{2/3} w_*^2\,, \tag{A.7}$$

$$F_i^{\mathrm{E}}(n) = \frac{S_i^{\mathrm{E}}(n)}{\sigma_i^2} = \frac{1}{(fm)_i}\frac{z}{U\,q}\left[1+\frac{1.5}{(fm)_i}\frac{f}{q}\right]^{-5/3}\,. \tag{A.8}$$

Substituting (A.6), (A.8) and $\beta_i = 0.55U/\sigma_i$ [30-32] into (A.3) yields

$$K_\alpha = \frac{0.09\,c_i^{1/2}\psi^{1/3}}{(fm)_i^{4/3}\,q^{4/3}}\frac{z^{4/3}}{z_i^{1/3}}w_*\int_0^\infty\frac{\sin(a\,n)}{\left[1+\frac{1.5\,n\,z}{(fm)_i\,U\,q}\right]^{5/3}}\frac{\mathrm{d}n}{n}\,, \tag{A.9}$$

where now the following terms in (A.3) are

$$\frac{\sigma_i^2\,\beta_i}{2\pi} = \frac{0.09\,U\,c_i^{1/2}w_*}{(fm)_i^{1/3}}\left(\frac{\psi}{q}\right)^{1/3}\left(\frac{z}{z_i}\right)^{1/3}\,, \tag{A.10}$$

and

$$\frac{2\pi t}{\beta_i} \equiv a = 11.76\frac{c_i^{1/2}}{(fm)_i^{1/3}}\left(\frac{\psi}{q}\right)^{1/3}\left(\frac{z}{z_i}\right)^{1/3}\frac{z_i}{U}X\,. \tag{A.11}$$

where $X = x\,w_*\,/\,U\,z_i$ can be thought of a non-dimensional time since it is the ratio of travel time x/U and the convective timescale z_i/w_*. Now define

$$n' = bn\,, \qquad \text{where } b = \frac{1.5\,z}{(fm)_i\,U\,q}\,. \tag{A.12}$$

Equation (A.9) can be written as

$$\frac{K_\alpha}{w_* z_i} = \frac{0.09\, c_i^{1/2} \psi^{1/3} (z/z_i)^{4/3}}{(fm)_i^{4/3}\, q^{4/3}} \int_0^\infty \frac{\sin\left(\frac{a}{b} n'\right)}{[1+n']^{5/3}} \frac{\mathrm{d}n'}{n'} \,, \tag{A.13}$$

and finally, like was firstly derived by Degrazia [15],

$$\frac{K_\alpha}{w_* z_i} = \frac{0.09\, c_i^{1/2} \psi^{1/3} (z/z_i)^{4/3}}{(fm)_i^{4/3}\, q^{4/3}} \int_0^\infty \frac{\sin\left[\dfrac{7.84\; c_i^{1/2}\, \psi^{1/3}\, (fm)_i^{1/3}\, q^{2/3}\, n'\, X}{(z/z_i)^{2/3}}\right]}{[1+n']^{5/3}\, n'} \frac{\mathrm{d}n'}{n'} \,. \tag{A.14}$$

Equation (A.14) contains the unknown function ψ. This mean dissipation of energy is important to quantify dispersion parameters since the order of magnitude of ψ is determined only by those quantities wich characterize the large eddies. Based on the Minnesota and Aschurch experiments [19], the dissipation function can be described as follows [24]:

$$\psi = 1.5 - 1.2 (z/z_i)^{1/3}. \tag{A.15}$$

For elevated releases we consider homogeneous turbulence so that the spectral peak wavelength can be written as $(\lambda_m)_w = z_i$ in order to obtain

$$q = \frac{(fm^*)_w}{(fm)_w} = \frac{z}{(\lambda_m)_w\, 0.35} = 2.86 \frac{z}{z_i} \,, \tag{A.16}$$

where $(fm)_w$ is equal to 0.35 [33]. To proceed, the vertical eddy diffusivity can be obtained from eqs. (A.14) and (A.16), using $c_w = 0.36$ and $(fm)_w = 0.35$ and be expressed as

$$\frac{K_z}{w_* z_i} = 0.054\, \psi^{1/3} \int_0^\infty \frac{\sin[4.71\, \psi^{1/3}\, X\, n']}{[1+n']^{5/3}\, n'} \mathrm{d}n' \,. \tag{A.17}$$

Equation (A.17) is the vertical eddy diffusivity depending on the source distance used in the present work. The asymptotic behavior of eq. (A.3) for large diffusion travel times ($t \to \infty$), when the eddy diffusivity has lost its memory of initial conditions is [34]

$$K_\alpha = \frac{\sigma_i^2\, \beta_i F_i^{\mathrm{E}}(0)}{4} \,. \tag{A.18}$$

Expression (A.18) together with $\beta_i = 0.55 (U/\sigma_i)$ and eqs. (A.6) and (A.8) leads to

$$K_\alpha = \frac{0.55}{4} \frac{\sigma_i\, z}{(fm)_i\, q} \,. \tag{A.19}$$

Finally, from (A.16) for the vertical eddy diffusivity there yields

$$\frac{K_z}{w_* z_i} = 0.085\, \psi^{1/3} \,. \tag{A.20}$$

Equation (A.20) is the vertical eddy diffusivity independent of the source distance used in the present work.

Finally, it is important to notice that the stability function q gives the frequency related to the maximum energy of spectral peak. For non-homogeneous turbulence $(\lambda_m)_w$ will be a function of the height and in consequence the function q and K will depend on the height. By the choice of $(\lambda_m)_w = z_i$ (homogeneous turbulence case) the z dependence in the vertical eddy diffusivities (eqs. (A.16) and (A.17)) disappears.

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