DERIVATION OF AN EDDY DIFFUSIVITY DEPENDING ON SOURCE DISTANCE UNDER MODERATELY UNSTABLE CONDITIONS

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ABSTRACT

Accounting for the current knowledge of the Convective Boundary Layer (CBL) structure and characteristics, a new formulation for eddy diffusivities has been derived, to be used in atmospheric dispersion models. Expressions are proposed for eddy diffusivities depending on source distance for inhomogeneous turbulence calculated directly with the Batchelor theory. The classical statistical diffusion theory, the observed spectral properties and the observed characteristics of energy-containing eddies are used to estimate these parameters. In addition, a vertical eddy diffusivity was introduced in an air pollution model and validated with the data of Copenhagen experiments and compared with the results of the obtained from classic formulation of the literature. A statistical evaluation show that, the results of the dispersion model with the K-parameterisation included, produces a good fit of the measured ground-level concentration data in the experimental conditions considered. Furthermore, the current work suggests that wind and eddy diffusivities profiles physically more realistic are important in regions near of an elevated source, and improves the description of the transport process of atmospheric pollutants.

Keywords: eddy diffusivity; analytical model; inhomoheneous turbulence; Planetary Boundary Layer.

RESUMO

Considerando-se o atual conhecimento sobre a estrutura e as características da Camada Limite Convectiva (CLC), foi obtida uma nova formulação geral para coeficientes de difusão para serem utilizados em modelos de dispersão atmosférica. Expressões são propostas para coeficientes de difusão dependentes da distância da fonte para turbulência não-homogênea, obtidas diretamente com a teoria de Batchelor. A teoria estatística de difusão clássica, as propriedades espectrais observadas e as características dos turbilhões mais energéticos são usados para estimar estes parâmetros. Além disso, o coeficiente de difusão vertical foi introduzido em um modelo de poluição do ar e validado com os dados experimentais de Copenhagen, além de comparado aos resultados de uma formulação clássica da literatura. Uma avaliação estatística mostra que os resultados do modelo de dispersão, utilizando a parametrização proposta, fornecem uma boa concordância com os dados de concentração superficiais nas condições experimentais consideradas. Adicionalmente, este trabalho sugere que perfis de vento e coeficientes de difusão mais reais são importantes em regiões próximas a uma fonte elevada, e melhoram a descrição do processo de transporte de poluentes atmosféricos.

Palavras-chave: coeficiente de difusão; modelo analítico; turbulência não-homogênea; Camada Limite Planetária.

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INTRODUCTION

The advection-diffusion equation has been largely applied in operational atmospheric dispersion models to predict mean concentrations of contaminants in the Planetary Boundary Layer (PBL). In principle, from this equation it is possible to obtain a theoretical model of dispersion from a continuous point source given appropriate boundary and initial conditions plus a knowledge of the mean wind velocity and concentration turbulent fluxes.

Much of the turbulent dispersion researches are related to the specification of these turbulent fluxes in order to allow the solution of the averaged advection-diffusion equation: this procedure, sometimes, is called as the closure of the turbulent diffusion problem. The main scheme for closing the equations is to relate concentration turbulent fluxes to the gradient of the mean concentration by eddy diffusivities, which are properties of the turbulent flow but not of the fluid; i.e. first-order closure (ARYA, 1995).

In the atmospheric diffusion problems the choice of a turbulent parameterisation represents a fundamental decision for the contaminants dispersion modeling. From a physical point of view a turbulence parameterisation is an approximation to nature in the sense that we are putting in mathematical models an approximated relation that in principle can be used as a surrogate for the natural true unknown term. The reliability of each model strongly depends on the way as turbulent parameters are calculated and related to the current understanding of the PBL.

The eddy diffusivity calculated by Batchelor (1949) can be identified as the coefficients of the advection-diffusion equation when it is considered a homogeneous turbulent flow. Although the diffusion coefficients presented by Batchelor (1949) were deduced originally for a homogeneous and stationary turbulent flow, they are used in regimes of stability that do not admit a homogeneity (case of the CBL) and they have if shown valid, because when used in dispersion models produce good results (MOREIRA et al., 1999; DEGRAZIA et al., 2001; MANGIA et al., 2002).

In the present work the eddy diffusivities are calculated directly with the Batchelor theory. This procedure allows to determine the eddy diffusivities in a simple and direct way. The derivation uses the classical statistical diffusion theory, the observed spectral properties and observed characteristics of the energy-containing eddies. These eddy diffusivities, derived for convective and moderately unstable conditions, contain the characteristic velocity and length scales of energy-containing eddies and can describe dispersion in the near and intermediate fields of an elevated continuous point source, i.e., when the scale of the plume is smaller than the scale of the turbulence. The resulting parameterised vertical eddy diffusivity is applied in the dispersion model Eulerian (MOREIRA; DEGRAZIA; VILHENA, 1999) to determine the concentration field generated by a height point source during the experiment of Copenhagen (GRYNING; LYCK, 1984) and compared with the results of the obtained from classic formulation of the literature (HANNA, 1982).

A MODEL FOR EDDY DIFFUSIVITIES

Following Batchelor (1949) and Taylor (1921) we can write:

$$K_{i,j} = \frac{1}{2}\frac{d\sigma^2}{dt} = \int_0^t R_{i,j}(\tau)d\tau \tag{1}$$

where the function correlation is defined as,

$$R_{i,j}(\tau) = \overline{u_i(t)u_j(t+\tau)} \tag{2}$$

The spectrum tensor $\Phi_{ij}(\omega)$, which is the Fourier transform of $R_{i,i}(\tau)$, is given by:

$$\Phi_{i,j}(\omega) = \int R_{i,j}(\omega)e^{-ikr}dr \tag{3}$$

$$R_{i,j}(\tau) = \int \Phi_{i,j}(\omega)e^{i\omega\tau}d\omega \tag{4}$$

By substituting equation (4) into equation (1), the following expression for eddy diffusivities is obtained:

$$K_{i,i} = \int_0^\infty \Phi_{i,i}(\omega)\frac{sin(\omega t)}{\omega}d\omega\,, \tag{5}$$

where it was considered that $\Phi_{ij}(\omega)$ is an even function in stationary field and, because of the interest in the sum of diagonal components of $\Phi_{ij}(\omega)$, it was considered $i = j$. As we are interested in expressing the diffusivity eddy as a function of the distance from the source, we can write the spectrum tensor in terms of the wave-number ($\Phi_{i,i}(\omega) = U\varphi_{i,i}(k)$). Besides, we will consider the function spectrum of energy $E(k) = 2\pi k^2\varphi_{i,i}(k)$, obtained by integrating the spectrum tensor over a spherical shell of radius k in wave-number space. We can write the equation (5) in the following form:

$$K_\alpha = \int_0^\infty E_\alpha(k)\frac{sin(kx)}{k}dk \qquad \alpha = x, y, z\ , \tag{6}$$

where $K_{1,1}, K_{2,2}, K_{3,3}$ is K_x, K_y, K_z, respectively and *x* is the distance of the source in meters.

From the Taylor (1921) theory, the dispersion parameters σ_α, determine the law that governs the average distribution of particles initially concentrated at one point, at any subsequent time. So, for the eddy diffusivities described by the equation (6) to be in agreement with the theory of Taylor, it is necessary to consider a reference system moving in the same velocity of the medium wind U. Therefore, the function spectrum of energy $E_\alpha(k)$ should be Lagrangian. However, as the spectra one-dimension are measured usually in fixed points, it is convenient to express the eddy diffusivities in terms of the spectrum Eulerian. Therefore, the eddy diffusivities coefficient are obtained of the general form:

$$K_\alpha = \frac{\beta_i}{U}\int_0^\infty E_\alpha^E(k)\frac{sin(kx/\beta_i)}{k}dk \quad i = u, v, w \quad , \quad (7)$$

where β_i is defined as the ratio of the Lagrangian to the Eulerian integral time scales.

THE VERTICAL EDDY DIFFUSIVITY

To calculate the vertical eddy diffusivity, considered to be the vertical component of the spectrum Eulerian of Degrazia e outros (1998):

$$E_w(k) = \frac{a_w}{(1 + b_w k)^{5/3}} \quad (8)$$

$$a_w = \frac{1.06}{2\pi}c_w\left(\frac{z}{z_i}\right)^{5/3} z_i \Psi^{2/3} w_*^2 \left[\left(f_m^*\right)_w^c\right]^{-5/3} \quad (8a)$$

$$b_w = \frac{1.5}{2\pi}\frac{z}{z_i}z_i\frac{1}{\left(f_m^*\right)_w^c}, \quad (8b)$$

where $c_w = 0.36$ (CHAMPAGNE et al., 1977); *z* is the height above the ground; z_i is the boundary layer height, w_* is the convective velocity scale; $\Psi = \frac{\varepsilon z_i}{w_*^3}$ is the dimensionless molecular dissipation rate function, where *e* is the mean dissipation of turbulent kinetic energy per unit time per unit mass of fluid; $\left(f_m^*\right)_w^c = \frac{z}{B_w z_i}$ is the normalized frequency of the spectral peak regardless of stratification, where:

$$B_w = 1.8\left[1 - \exp\left(-\frac{4z}{z_i}\right) - 0.0003\exp\left(\frac{8z}{z_i}\right)\right],$$

is the value of the vertical wavelength at the spectral peak, which was obtained from empirical data by Caughey & Palmer (1979).

To calculate the vertical eddy diffusivity from equation (7) we considered $\beta_w = 0.55\frac{U}{\sigma_w}$ (WANDEL; KOFOED-HANSEN, 1962; CORSIN, 1963; DEGRAZIA; ANFOSSI, 1998), where:

$$\sigma_w^2 = \int_0^\infty E_w(k)dk, \quad (9)$$

is the variance of the vertical component of the velocity.

Then, the vertical eddy diffusivity described in terms of energy-containing eddies, function of the dimensionless distance $X = xw_*/Uz_i$ and the dimensionless height z/z_i can be written as:

$$\frac{K_z}{w_* z_i} = 0.054\left(\frac{z/z_i}{\left(f_m^*\right)_w^c}\right)^{4/3}\Psi^{1/3}\int_0^\infty \frac{sin\left(1.12(z/z_i)^{1/3}\left[\left(f_m^*\right)_w^c\right]^{-1/3}\Psi^{1/3}Xz_i k\right)}{\left(1 + \frac{1.5}{2\pi}\frac{z}{\left(f_m^*\right)_w^c}k\right)^{5/3}}\frac{dk}{k} \quad (10)$$

Eq. (10) contains the unknown function Ψ. This molecular dissipation of turbulent velocity is one of the leading destruction terms in equations for the budget of second-order moments. Therefore, the PBL evolution is dependent on this function. Observations and numerical simulations in central regions of the CBL show that $\Psi \cong 0.4$ (CAUGHEY, 1982; MOENG; WYNGAARD, 1989; SCHMIDT; SHUMANN, 1989). Nevertheless, several field experiments in a CBL (KAIMAL et al., 1976; CAUGHEY, 1982; LENSCHOW; WYNGAARD; PENNEL, 1980) emphasize that for dimensionless heights in the range $0.05 < z/zi < 0.3$ the values of Ψ are much greater than 0.4. Following DRUILHET e outros (1983), the profile Ψ can be approximated by the exponential law:

$$\Psi = 1.26\exp\left[-\frac{z}{0.8z_i}\right] \quad (11)$$

On the other hand, based on the Minnesota and Aschuerch experiments (Caughey, 1982), the dissipation function can be described as follows (LUHAR; BRITTER, 1989):

$$\Psi = 1.5 - 1.2(z/z_i)^{1/3} \quad (12)$$

Finally, Hfjstrup (1982) suggested the following fitting curve for the dissipation rate of turbulent kinetic energy:

$$\Psi = \left[\left(1 - \frac{z}{z_i}\right)^2\left(\frac{z}{-L}\right)^{-2/3} + 0.75\right]^{3/2}, \quad (13)$$

where *L* is the Monin-Obukhov length in the surface layer.

For comparison and evaluation of the parameterisation dependent of *x* and *z* proposed in this work will use the proposal for Hanna (1982) that is only dependent of the height *z* and is widely used in pollutant dispersion models. This parameterisation describes the turbulence field from the surface layer and boundary layer parameters z_0, L, u_*, w_*, h and z_i. Hanna suggested, from Minnesota PBL observations, different expressions for the variances (σ_w) and for the Lagrangian time scales (T_{L_w}) distinguishing the different kind of atmospheric stratification conditions, the unstable, stable and neutral cases. For the unstable case, the expressions for σ_i^2 and τ_{Li} are the following:

$$\frac{\sigma_w}{w_*} = 0.90\left(3\frac{z}{z_i} - \frac{L}{z_i}\right)^{1/3} \quad \frac{z}{z_i} < 0.03 \tag{14a}$$

$$\frac{\sigma_w}{w_*} = min\left[0.96\left(3\frac{z}{z_i} - \frac{L}{z_i}\right)^{1/3}, 0.763\left(\frac{z}{z_i}\right)^{0.175}\right]$$

$$0.03 < \frac{z}{z_i} < 0.4 \tag{14b}$$

$$\frac{\sigma_w}{w_*} = 0.722\left(1 - \frac{z}{z_i}\right)^{0.207} \quad 0.4 < \frac{z}{z_i} < 0.96 \tag{14c}$$

$$\frac{\sigma_w}{w_*} = 0.37 \quad 0.96 < \frac{z}{z_i} < 1 \tag{14d}$$

$$T_{L_w} = 0.1\frac{z}{\sigma_u}\frac{1}{\left(0.55 + 0.38(z - z_o)/L\right)}$$

$$\frac{z}{z_i} < 0.1, \; -\frac{(z - z_o)}{L} < 1 \tag{15a}$$

$$T_{L_w} = 0.59\frac{z}{\sigma_w} \quad \frac{z}{z_i} < 0.1, \; -\frac{(z - z_o)}{L} > 1 \tag{15b}$$

$$T_{L_w} = 0.15\frac{z_i}{\sigma_w}\left(1 - exp\left(-5\frac{z}{z_i}\right)\right) \quad \frac{z}{z_i} > 0.1 \tag{15c}$$

where K_z is given by the relation:

$$K_z = \sigma_w^2 T_{L_w} \tag{16}$$

Thus, in this study we introduce the vertical eddy diffusivities (10) and (16) in an air pollution model to simulate the ground-level crosswind-integrated concentrations of contaminants released from an elevated continuous source in an moderately unstable PBL.

AIR POLLUTION MODEL

Following Vilhena (VILHENA et al., 1998; MOREIRA; DEGRAZIA; VILHENA, 1999; DEGRAZIA; MOREIRA; VILHENA, 2001; MANGIA et al., 2002), for a cartesian coordinate system in which the *x* direction coincides with that of the average wind, the steady-state advection-diffusion equation is written as in Arya (1995):

$$U\frac{\partial \bar{c}}{\partial x} = \frac{\partial}{\partial x}\left(K_x\frac{\partial \bar{c}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial \bar{c}}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial \bar{c}}{\partial z}\right), \tag{14}$$

where $\bar{c}$ denotes the average concentration, *U* the mean wind speed in *x* direction and K_x, K_y and K_z are the eddy diffusivities. The cross-wind integration of the equation (14) (neglecting the longitudinal diffusion) leads to:

$$U\frac{\partial \overline{c^y}}{\partial x} = \frac{\partial}{\partial z}\left(K_z\frac{\partial \overline{c^y}}{\partial z}\right), \tag{15}$$

subjected to the boundary conditions of zero flux at the ground and PBL top, and a source with emission rate *Q* at height H_s:

$$K_z\frac{\partial \overline{c^y}}{\partial z} = 0 \text{ at } z = 0, z_i \tag{16}$$

$$U\overline{c^y}(0,z) = Q\delta(z - H_s) \text{ at } x = 0, \tag{17}$$

where now $\overline{c^y}$ represents the average crosswind integrated concentration.

Bearing in mind the dependence of the K_z coefficient and wind speed profile *U* on variable *z*, the height z_i of a CBL is discretized in *N* sub-intervals in such a manner that, inside each interval, $K_z(z)$ and $U(z)$ assume, respectively, the average value:

$$K_n = \frac{1}{z_{n+1} - z_n}\int_{z_n}^{z_{n+1}} K_z(z)dz \tag{18}$$

$$U_n = \frac{1}{z_{n+1} - z_n}\int_{z_n}^{z_{n+1}} U(z)dz \tag{19}$$

For the vertical eddy diffusivity depending on *x* and *z*, initially we take the average, in the *z* variable:

$$K_n(x) = \frac{1}{z_{n+1} - z_n}\int_{z_n}^{z_{n+1}} K_z(x,z)dz \tag{20}$$

The procedure is quite similar for the x variable. Indeed, the domain in the x variable is discretized into variable sub-intervals of length Δx_i and in each sub-interval, the following average value for the eddy diffusivity is considered:

$$K_{i,n} = \frac{1}{x_{i+1} - x_i} \int_{x_i}^{x_{i+1}} K_n(x')dx' \qquad (21)$$

Recall that $K_{i,n}$ assumes a constant value at $x_i \leq x \leq x_{i+1}$ and $z_n \leq z \leq z_{n+1}$.

Therefore, the solution of problem (15) is reduced to the solution of N problems of the type:

$$U_n \frac{\partial \overline{c_n^y}}{\partial x} = K_{i,n} \frac{\partial^2 \overline{c_n^y}}{\partial z^2} \quad z_n \leq z \leq z_{n+1}, \; x_i \leq x \leq x_{i+1} \quad (22)$$

for $n = 1$: N, where $\overline{c_n^y}$ denotes the concentration at the n^{th} sub-interval. To determine the $2N$ integration constants the additional ($2N$-2) conditions namely continuity of concentration and flux at interface are considered:

$$\overline{c_n^y} = \overline{c_{n+1}^y} \quad n = 1, 2,...(N-1) \qquad (23)$$

$$K_n \frac{\partial \overline{c_n^y}}{\partial z} = K_{n+1} \frac{\partial \overline{c_{n+1}^y}}{\partial z} \quad n = 1, 2,...(N-1) \qquad (24)$$

Applying the Laplace transform in equation (22) results:

$$\frac{\partial^2}{\partial z^2} \overline{c_n^y}(s,z) - \frac{U_n s}{K_n} \overline{c_n^y}(s,z) = -\frac{U_n}{K_n} \overline{c_n^y}(0,z) \quad , (25)$$

where $\overline{c_n^y}(s,z) = L_p \left\{ \overline{c_n^y}(x,z); x \to s \right\}$, which has the well-know solution:

$$\overline{c_n^y}(s,z) = A_n e^{-R_n z} + B_n e^{R_n z} + \frac{Q}{2R_a} \left(e^{-R_n (z-H_s)} - e^{R_n (z-H_s)} \right) \quad ,(26)$$

where:

$$R_n = \pm \sqrt{\frac{U_n s}{K_n}} \text{ and } R_a = \pm \sqrt{U_n K_n s}$$

Finally, applying the interface and boundary conditions we come out with a linear system for the integration constants. Henceforth, the concentration is obtained inverting numerically the transformed concentration c^y by Gaussian quadrature scheme (HEYDARIAN; MULLINEAUX, 1989):

$$\overline{c_n^y}(x,z) = \sum_{j=1}^{8} A_j \frac{P_j}{x} \left(A_n e^{-\left(\sqrt{\frac{P_j U_n}{x K_n}}\right) z} + B_n e^{\left(\sqrt{\frac{P_j U_n}{x K_n}}\right) z} \right) \qquad (27)$$

$$\overline{c_n^y}(x,z) = \sum_{j=1}^{8} A_j \frac{P_j}{x} \left[A_n e^{-\left(\sqrt{\frac{P_j U_n}{x K_n}}\right) z} + B_n e^{\left(\sqrt{\frac{P_j U_n}{x K_n}}\right) z} + \frac{1}{2} \frac{Q}{\sqrt{\frac{P_j K_n U_n}{x}}} \left(e^{-(z-H_s)\left(\sqrt{\frac{P_j U_n}{x K_n}}\right)} - e^{(z-H_s)\left(\sqrt{\frac{P_j U_n}{x K_n}}\right)} \right) \right] \qquad (28)$$

The solution (27) is valid for layers that do no contain the contaminant source. On the other hand, the solution (28) can be used to evaluate the concentration field in the layer that contains the continuous source. These solutions are only valid for $x > 0$, once the quadrature scheme of Laplace inversion doesn't work for $x = 0$. A_j and P_j are the weights and roots of the Gaussian quadrature scheme and are tabulated in the book by Stroud & Secrest (1966).

To this point, it is important to mention that this procedure leads to a solution for the concentration with a continuous dependence on z and is sectionally continuous on x because it was imposed the condition of continuity of concentration and flux concentration at the interface z_n. To get a solution with a continuous dependence on x and z variables, we must apply, besides the boundary conditions, the interface conditions of continuity of concentration at x_i and z_n. The justificative for the adopted approach stems from the simplicity resulting from the straight application of the formulation for concentration encountered by Moreira (2000), when the eddy diffusivity coefficient varies only along the z variable. Furthermore, no additional computational effort is required to evaluate the concentration when the eddy diffusivity depends on x and z. We are aware that this procedure is an approximation because of the discontinuity in concentration at the interface x_i, but it improves the results, as shown later on. It is also relevant to recall that for both approaches, the number of integration constants are equal to the number of boundary and interface conditions, consequently the integration constants are uniquely determined.

MODEL EVALUATION

The performance of the present model (Eqs. 10, 27, 28) have been evaluated against experimental ground-level concentration using tracer SF_6 data from dispersion experiments carried out in the northern part of Copenhagen, described in Gryning e outros (1987). The tracer was released without buoyancy from a tower at a height of 115 m, and collected at 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 1 shows the meteorological data from Gryning & Lyck (1984) and Gryning e outros (1987) utilized during the experiments that were used for the validation of the proposed approach. The mean wind speed measured at the released height and presented in Table 1 was used to calculate the vertical eddy diffusivity (Eq. 10) for each dispersion experiment. To calculate w_*, the relation $w_* / u_* = (-z_i / kL)^{1/3}$ was used. The Copenhagen data set was chosen since most of the experiments were performed during unstable moderately atmospheric conditions, and without strong buoyancy, so that the ground-level crosswind integrated concentration could be simulated by an advection-diffusion equation. The stability parameter z_i/L indicates cases where the unstable PBL presents weak to moderate convection.

Tabela 1 – Resumo das condições meteorológicas durante os experimentos

Table 1 – Summary of meteorological conditions during the experiments

Exp.	U (ms^{-1})	u_* (ms^{-1})	L (m)	w_* (ms^{-1})	z_i (m)
1	3.4	0.36	-37	1.8	1.980
2	10.6	0.73	-292	1.8	1.920
3	5.0	0.38	-71	1.3	1.120
4	4.6	0.38	-133	0.7	390
5	6.7	0.45	-444	0.7	820
6	13.2	1.05	-432	2.0	1.300
7	7.6	0.64	-104	2.2	1.850
8	9.4	0.69	-56	2.2	810
9	10.5	0.75	-289	1.9	2.090

The wind speed profile used in Eqs. (27) and (28) has been parameterized following the similarity theory of Monin-Obukhov and OML model (BERKOWICZ; OLESEN; TORP, 1986):

$$U = \frac{u_*}{k}\left[\ln(z/z_0) - \Psi_m(z/L) + \Psi_m(z_0/L)\right] \text{ if } z \leq z_b \quad (29)$$

$$U = U(z_b) \text{ if } z > z_b\,, \quad (30)$$

where $z_b = \min[|L|, 0.1 z_i]$, and Ψ_m is a stability function given by (Paulsen, 1975):

$$\Psi_m = 2\ln\left[\frac{1+A}{2}\right] + \ln\left[\frac{1+A^2}{2}\right] - 2\tan^{-1}(A) + \frac{\pi}{2}\,, \quad (31)$$

with:

$$A = (1 - 16z/L)^{1/4}\,, \quad (32)$$

$k = 0.4$ is the Von Karman constant, u_* is the friction velocity and z_o roughness length.

As a test for the approach (10), (27) and (28) and also to analyze the influence of the memory effect in the turbulent transport the parameterization (10), with ψ given by Eqs. (11), (12) and (13), are used to simulate the ground-level crosswind integrated concentrations $c^y(x,0)$ of Copenhagen. Figure 1 shows the observed and predicted scatter diagram of ground-level crosswind concentrations using the approach (27) and (28) with vertical eddy diffusivities given by Eq. (10) and (16). In this respect, it is important to note that a better fitting was encountered for the values of the eddy diffusivity $K_z(x,z)$ evaluated by Eq. (10) with the Eq. (11). The simulation using in the K-model the parameterisation of Hanna (1982) tends to overestimate the concentrations.

Figure 2 shows the behavior of vertical profiles of K_z as given by Eq. (10). Particularly for Eq. (10) vertical profiles are plotted for three different distances from the source ($x = 2000$, 4000 and 6000 m). Each profile represents a well-behaved eddy diffusivity with a maximum in the central regions of the CBL and with small values at $z = 0$ and $z = z_i$. The behavior of the vertical eddy diffusivity for two different heights ($z/z_i = 0.1$ and $z/z_i = 0.5$), as given by Eq. (10), as a function of the nondimensional distance X, is presented in Figure 3. We can observe from these figures that, for various distances X involved in the Copenhagen experiment, the K_z aymptotic value is not reached. As a consequence, Eq. (10) represents a formula appropriate to describe dispersion in the near and intermediate fiels of an elevated source.

Table 2 presents some measures performances obtained by using the statistical evaluation procedure described by Hanna (1989) and defined in the following way:

Nmse (normalized mean square error) $= \overline{(C_o - C_p)^2} / \overline{C_o}\,\overline{C_p}$,

Fa2 = fraction of data (%) for $0.5 \leq (C_p / C_o) \leq 2$

Cor (correlation coefficient) $= \overline{(C_o - \overline{C_o})(C_p - \overline{C_p})} / \sigma_o \sigma_p$,

Fb (fractional bias) $= \overline{C_o} - \overline{C_p} / 0.5(\overline{C_o} + \overline{C_p})$,

Fs (fractional standard deviations) $(\sigma_o - \sigma_p)/0.5(\sigma_o + \sigma_p)$

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

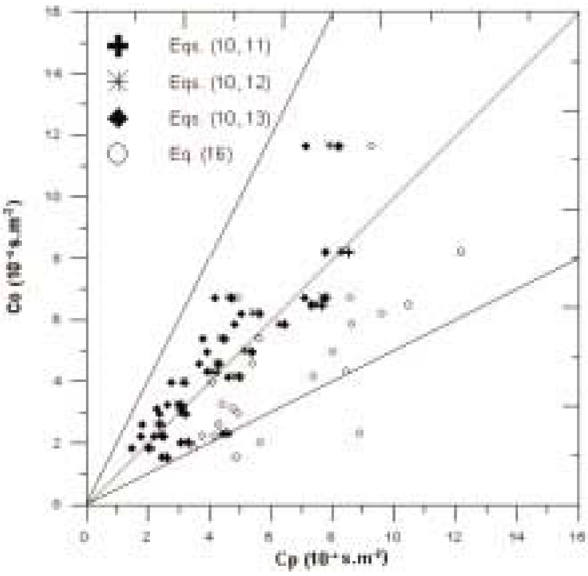

Figura 1 – Diagrama de espalhamento das concentrações superficiais integradas lateralmente observadas (Co) e preditas (Cp), normalizadas com a taxa de emissão ($\overline{c^y}/Q$) para a solução das eqs. (10, 11, 27, 28), eqs. (10, 12, 27, 28), eqs. (10, 13, 27, 28) e eqs. (16, 27, 28).

Figure 1 – Observed (Co) and predicted (Cp) crosswind ground level integrated concentration, normalised with emission ($\overline{c^y}/Q$), scatter diagram for the solution of eqs. (10, 11, 27, 28), eqs. (10, 12, 27, 28), eqs. (10,13, 27, 28) and eqs. (16, 27, 28).

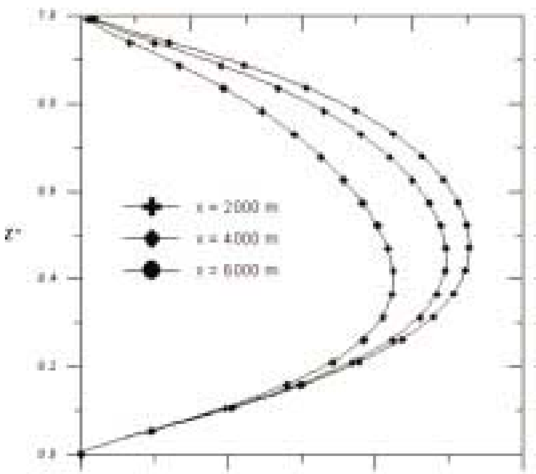

Figura 2 – O comportamento do perfil vertical para o coeficiente de difusão dependente da distância da fonte para três distâncias diferentes (x = 2000 m, x = 4000 m and x = 6000 m, Eq. 10, $Z^* = z / z_i$ e $K^* = K_z / w_* z_i$).

Figure 2 – The behaviour of the vertical profile for the eddy diffusivity depending on source distance for three different distances (x = 2000 m, x = 4000 m and x = 6000 m, Eq. 10, $Z^* = z / z_i$ and $K^* = K_z / w_* z_i$).

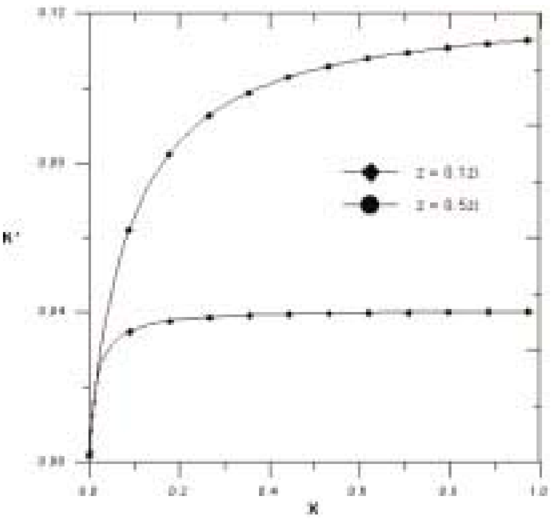

Figura 3 – O comportamento do coeficiente de difusão vertical ($K^* = K_z / w_* z_i$) para duas diferentes alturas ($z/z_i = 0.1$ e $z/z_i = 0.5$), dado pela eq. (10), em função da distância adimensional *X*.

Figure 3 – The behaviour of the vertical eddy diffusivity ($K^* = K_z / w_* z_i$) for two different heights ($z/z_i = 0.1$ and $z/z_i = 0.5$), as given by eq. (10), in function of the nondimensional distance X.

Tabela 2 – Índices estatísticos da performance dos modelos
Table 2 – Statistical indices used to evaluate the model performance

Model	Nmse	Fa2	Cor	Fb	Fs
Eqs. (27, 28, 10, 11)	0.06	1.00	0.90	-0.02	-0.01
Eqs. (27, 28, 10, 12)	0.06	1.00	0.89	-0.06	-0.01
Eqs. (27, 28, 10, 13)	0.10	1.00	0.87	-0.11	-0.19
Eqs. (27, 28, 16)	0.28	0.87	0.68	-0.38	-0.02

The statistical evaluation highlight a quite satisfactory performance obtained with the proposed approach that considers the K_z value to vary with the distance from source. In particular, when the model utilise the dissipation rate of turbulent kinetic energy represented by the Eq. (11) the performance is better; Fa2 is 100%, Cor is 90% and low Fs and Fb (closer of zero).

CONCLUSIONS

A general method to derive eddy diffusivities depending on source distance calculated directly with the Batchelor theory for a turbulent moderately unstable PBL is proposed. This method is based upon a model for the spectra of the turbulent kinetic energy and the Taylor statistical diffusion theory. These coefficients are valid in the near, intermediate and far field of an elevated source. The integral form of the eddy diffusivity (Eq. 10) is more complicated than the algebraic one available in the literature. On the other hand is is more general since, unlike the algebraic parameterisations, it does not utilize turbulent dispersion measurements. The present model provides a vertical eddy diffusivity varying with distance from the source for inhomogeneous turbulence in a CBL (K_z is dependent on the dimensionless distance, $X = xw_*/Uz_i$ and is also dependent on the height z/z_i) that was introduced in an air pollution model and validated with the data of Copenhagen experiments (GRYNING; LYCK, 1984). The statistical analysis of the results shows a good agreement between the results of the proposed approach with the experimental ones. The current work suggests that wind and eddy diffusivities profiles physically more realistic are important in regions near of an elevated source, and improves the description of the transport process of atmospheric pollutants.

Finally, it is relevant to mention that the proposed model for eddy diffusion coefficient, expressed by (Eq. 10), depending on source distance and valid for an inhomogeneous turbulence is suitable for application in diffusion atmospheric models.

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