An air pollution model with eddy diffusivities depending on source distance considering atmospheric turbulence generated by mechanical and thermal forcing

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1. Introduction

The advection-diffusion equation has been largely applied in operational atmospheric dispersion models to predict mean concentrations of contaminants in the Atmospheric Boundary Layer (ABL). 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 knowledge of the mean wind velocity and concentration turbulent fluxes. 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). Even more important, the eddy diffusivities may vary in space and with the travel time of contaminants. In his statistical diffusion theory, Taylor (1921) pointed out that turbulent diffusion differs in the near and the far regions from a continuous point source. In the proximity of the source, fluid particles retain their memory of their initial turbulent environment. For long travel times, this memory is lost, and particles follow only the local properties of turbulence (Batchelor, 1949).

The aim of this work is to report a mathematical model describing the crosswind-integrated concentrations for dispersion of pollutants emitted from a continuous source in the atmospheric boundary layer. It considers the wind speed as a function of vertical height above the ground surface and eddy diffusivity as a function of both downwind distance from the source and vertical height. Besides, an integral parameterization of the vertical eddy diffusivity in a shear–buoyancy-driven atmospheric boundary layer is developed by using a model for the frequency spectrum of eddy energy in the surface layer. Expressions of eddy diffusivities for vertically inhomogeneous turbulence and also dependent on source distance are proposed, which are calculated directly with the Batchelor's theory and further developments suggested by Hojstrup and Monin-Obukhov scaling (Panofsky and Dutton, 1984). The statistical independence of Fourier components for distant frequencies allows the specification of the turbulent kinetic energy spectrum as the sum of buoyancy and a shear-produced part. The model and the new eddy diffusivities are well suited for application in air pollution modeling under unstable/neutral conditions.

To reach this goal, we outline the paper as follows: in section 2, we report the derivation of the solution for the advection-diffusion equation with eddy diffusivities depending on x and z variables; in section 3 the turbulent parameterization assumed in this work is presented; in section 4, the wind speed profile is reported; finally, in section 5 we present discussions with future perspectives.

2. An air pollution model

For a Cartesian coordinate system in which the x direction coincides with that one of the average wind, the steady state advection-diffusion equation is written as (Arya, 1995):

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

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 (17) (neglecting the longitudinal diffusion) leads to (Moreira and Vilhena, 2009):

$$U\frac{\partial \overline{c^y}}{\partial x} = \frac{\partial}{\partial z}\left(K_z \frac{\partial \overline{c^y}}{\partial z}\right) \tag{2}$$

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

$$K_z \frac{\partial \overline{c^y}}{\partial z} = 0 \quad \text{at} \quad z = 0, z_i \tag{3}$$

$$U\overline{c^y}(0,z) = Q\delta(z - H_s) \qquad \text{at} \quad x = 0 \tag{4}$$

where now $\overline{c^y}$ represents the average cross-wind 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 ABL is discretized in N sub-intervals in such a manner that inside each interval $K_z(z)$ and $U(z)$ assume the average value:

$$K_n = \frac{1}{z_{n+1} - z_n}\int_{z_n}^{z_{n+1}} K_z(z)dz \tag{5}$$

$$U_n = \frac{1}{z_{n+1} - z_n}\int_{z_n}^{z_{n+1}} U(z)dz \tag{6}$$

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

$$\overline{K}_n(x) = \frac{1}{z_{n+1} - z_n}\int_{z_n}^{z_{n+1}} K_z(x,z)dz \tag{7}$$

Recall that K_n assumes a constant value at $z_n \le z \le z_{n+1}$. Therefore the solution of problem (2) is reduced to the solution of N problems of the type:

$$U_n \frac{\partial \overline{c_n^y}}{\partial x} = \overline{K}_n(x)\frac{\partial^2 \overline{c_n^y}}{\partial z^2} \qquad z_n \le z \le z_{n+1} \tag{8}$$

for n = 1: N, where $\overline{c_n^y}$ denotes the concentration at the n^{th} sub-interval.

Here we have the first novelty of this work. To obtain the solution of Eq. (8), we make a change of variables (Crank, 1979):

$$U_n \frac{\partial \overline{c_n^y}}{\partial x^*} = \frac{\partial^2 \overline{c_n^y}}{\partial z^2} \tag{9}$$

where $x^* = \int_0^x \overline{K}_n(x)dx$.

To determine the $2N$ integration constants the additional ($2N$-2) conditions namely continuity of concentration and flux at interface are considered:

$$\overline{c_n^y} = \overline{c_{n+1}^y} \qquad n = 1, 2,...(\text{N-1}) \tag{10}$$

$$K_n \frac{\partial \overline{c_n^y}}{\partial z} = K_{n+1}\frac{\partial \overline{c_{n+1}^y}}{\partial z} \qquad n = 1, 2,...(\text{N-1}) \tag{11}$$

Applying the Laplace transform in equation (9) results:

$$\frac{\partial^2}{\partial z^2}\overline{c_n^y}(s,z) - U_n s\overline{c_n^y}(s,z) = -U_n \overline{c_n^y}(0,z) \tag{12}$$

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:

$$\overline{c_n^y}(s,z) = A_n e^{-R_n z} + B_n e^{R_n z} + \frac{Q}{2R_a}\left(e^{-R_n(z-H_s)} - e^{R_n(z-H_s)}\right) \tag{13}$$

where,

$$R_n = \sqrt{U_n s} \quad \text{and} \quad R_a = \sqrt{U_n s}$$

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 $\overline{c^y}$ by Gaussian quadrature scheme:

$$\overline{c_n^y}(x^*,z) = \sum_{j=1}^{8} A_j \frac{P_j}{x^*}\left[A_n e^{-\left(\sqrt{\frac{P_j U_n}{x^*}}\right)z} + B_n e^{\left(\sqrt{\frac{P_j U_n}{x^*}}\right)z} + \frac{1}{2}\frac{Q}{\sqrt{\frac{P_j U_n}{x^*}}}\left(e^{-(z-H_s)\left(\sqrt{\frac{P_j U_n}{x^*}}\right)} - e^{(z-H_s)\left(\sqrt{\frac{P_j U_n}{x^*}}\right)}\right)\right] \tag{14}$$

where A_j and P_j are the weights and roots of the Gaussian quadrature scheme and are tabulated in the book by Stroud and Secrest (1966).

3. A model for eddy diffusivities depending on height and source distance in the surface layer

A new integral parameterization of the vertical eddy diffusivity in a shear–buoyancy-driven atmospheric boundary layer can be developed by using a model for the frequency spectrum of eddy energy in the surface layer. The statistical independence of Fourier components for distant frequencies allows the specification of the turbulent kinetic energy spectrum as the sum of a buoyancy and a shear-produced part (Panofsky and Dutton, 1984). Hojstrup's model (Hojstrup, 1981) divides the spectra (nondimensional) into high and low frequency parts, as the sum of a buoyancy and a shear-produced, respectively:

$$S(n) = S_L(n) + S_H(n) \tag{15}$$

where the low frequency part $S_L(n)$ (bouyancy production) for the vertical component depends on $n = fz/U$ and z/L, where n a dimensionless frequency, f is the frequency, z is the height above the ground and U is the longitudinal wind speed. The high frequency part $S_H(n)$ (shear production) depends on function of $n = fz/U$. Specifically, the model contains the following expression for the vertical component:

$$\frac{fS_w(f)}{u_*^2} = \frac{32n}{(1+17n)^{5/3}}\left(\frac{z}{-L}\right)^{2/3} + \frac{2n}{1+5.3n^{5/3}} \tag{16}$$

where $S_w(f)$ is the spectral density of w. The surface friction velocity is represented by u_*. The vertical Eulerian turbulent velocity variance is written as:

$$\sigma_w^2 = \int_0^\infty S_w(f)df \tag{17}$$

The present approach fundamentally hinges on Batchelor’s (1949) time-dependent equation for the evolution of eddy diffusivities:

$$K_z = \frac{\beta_w}{2\pi}\int_0^\infty S_w(f)\sin(2\pi ft/\beta_w)\frac{df}{f} \tag{18}$$

where $\beta_w = \gamma \dfrac{U}{\sigma_w}$ is defined as the ratio of the Lagrangian to the Eulerian integral time scales in the vertical direction ($\gamma = 0.55$ is the Corrsin constant) and $t = x/U$ (travel time).

The vertical spectral density considering only buoyancy effect is:

$$S_{wb}(f) = \frac{32u_*^2 z}{U(1+17\, fz/U)^{5/3}}\left(\frac{z}{-L}\right)^{2/3} \tag{19}$$

Then, using Eq. (17), the vertical Eulerian turbulent velocity variance is:

$$\sigma_{wb}^2 = 2.82u_*^2\left(\frac{z}{-L}\right)^{2/3} \tag{20}$$

Using the relation for β_w results:

$$\beta_w = \frac{0.33}{u_*}U\left(\frac{z}{-L}\right)^{-1/3} \tag{21}$$

and, using Eq. (18), we obtain we obtain the vertical eddy diffusivity considering buoyancy effect in the surface layer:

$$\frac{K_z^b(x,z)}{u_* z} = 1.66\left(\frac{z}{-L}\right)^{1/3}\int_0^\infty \frac{\sin\left(19.21X\,(z/-L)^{1/3}\,n\right)}{(1+17n)^{5/3}}\frac{dn}{n} \tag{22}$$

where $X = \dfrac{u_* x}{Uz}$.

The vertical spectral density considering only shear effect is written as:

$$S_{ws}(f) = \frac{2u_*^2 z}{U\left[1+5.3(fz/U)^{5/3}\right]} \tag{23}$$

Then, using Eq. (17), the vertical Eulerian turbulent velocity variance is:

$$\sigma_{ws}^2 = 1.46u_*^2 \tag{24}$$

Using the relation for β_w results:

$$\beta_w = 0.46\frac{U}{u_*} \tag{25}$$

and, using Eq. (18), we obtain the vertical eddy diffusivity considering shear effect in the surface layer:

$$\frac{K_z^s(x,z)}{u_* z} = 0.15\int_0^\infty \frac{\sin(13.65Xn)}{(1+5.3n^{5/3})}\frac{dn}{n} \tag{26}$$

Finally, take into account the contribution of buoyancy and shear parts, combining the Eqs. (22) and (26), we have:

$$K_z(x,z) = K_z^b(x,z) + K_z^s(x,z) \tag{27}$$

It is important to mention that the x* variable, that include the resulting eddy diffusivity (27), is:

$$x^* = \int_0^x \bar{K}_z(x)dx = \int_0^x \left(\bar{K}_z^b(x) + \bar{K}_z^s(x)\right)dx \tag{28}$$

where

$$\bar{K}_z^b(x) = \frac{1}{z_{n+1}-z_n}\int_{z_n}^{z_{n+1}} K_z^b(x,z)dz \quad ; \quad \bar{K}_z^m(x) = \frac{1}{z_{n+1}-z_n}\int_{z_n}^{z_{n+1}} K_z^s(x,z)dz \tag{29}$$

The eddy diffusivity (27), as a function of downwind distance, is dependent of z and yields a description of turbulent dispersion in the near, intermediate and far fields of a source in the surface layer (the memory effect of turbulent transport is considered).

4. Vertical wind speed parameterization

The wind speed profile used in the Eq. (14) has been parameterized following the similarity theory of Monin-Obukhov and OML model (Berkowicz et al., 1986):

$$U = \frac{u_*}{k}\left[\ln(z/z_0) - \Psi_m(z/L) + \Psi_m(z_0/L)\right] \qquad \text{if } z \le z_b \tag{30}$$

$$U = U(z_b) \qquad \text{if } z > z_b \tag{31}$$

where $z_b = min\left[|L|, 0.1 z_i\right]$,and Ψ_m is a stability function given by (Paulson, 1970):

$$\Psi_m = 2\ln\left[\frac{1+A}{2}\right] + \ln\left[\frac{1+A^2}{2}\right] - 2\tan^{-1}(A) + \frac{\pi}{2} \tag{32}$$

with,

$$A = (1 - 16z/L)^{1/4} \tag{33}$$

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

5. Discussions and perspectives

In this work, we present an analytical solution of the two dimensional advection–diffusion equation by using integral transform method considering the eddy diffusivity depending on x and z variables. By analytical we mean that no approximation is made along its derivation. Analytical solutions are of fundamental importance in understanding and describing physical phenomena, since they are able to take into account all the parameters of a problem, and investigate their influence. Moreover, we need to remember that air pollution models have two kinds of errors. The first one is due to the physical modeling and another one inherent to the numerical solution of the equation associated to the model. Henceforth, we may affirm that the analytical solution, in some sense, mitigate the error associated to the mathematical model. As a consequence, the model errors somehow, restricts to the physical modeling error.

Besides, a method to derive eddy diffusivities depending on source distance for a turbulent unstable/neutral ABL was proposed. These coefficients are valid in the near, the intermediate and far field of a continuous source located in the surface layer. The present model provides a vertical eddy diffusivity varying with distance from the source for inhomogeneous turbulence (K_z is dependent on the nondimensional distance, $X = xu_*/Uz$ and is also dependent on the stability parameter z/L).

We focus our attention in the future to evaluate the memory effect and reinforce our confidence in the parameterization (27) with numerical comparisons using experimental dataset. Furthermore, it is important to emphasize that we will be verify if the results obtained with the eddy diffusivity depending on the source distance are better than the ones reached with asymptotic eddy diffusivity, valid only for the far field of a source.

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