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POLLUTANT DISPERSION MODELING IN LOW WIND AND STABLE CONDITIONS

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ABSTRACT

The aim of this work is to present an analytical solution to the three-dimensional advection-diffusion equation in low wind conditions in a stable boundary layer dominated by shear. The model includes the longitudinal diffusion that can not be neglected in low wind conditions. The solution of the advection-diffusion equation is obtained applying the integral transform technique. To validate this methodology, data collected during the classic Prairie Grass experiment were employed. To verify the performance of the model were utilized integral and algebraic eddy diffusivities to parameterize the turbulence. The wind profile is described by power and similarity law.

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INTRODUCTION

The importance of to study the pollutant dispersion in low wind and stable conditions lies in the fact that such situations frequently occurs in the Planetary boundary layer (PBL) and, therefore, we need to derive new dispersion models that describe this turbulent state of the PBL. In low wind conditions, the pollutants are not dispersed to far from the source, because of the low wind magnitude and the near-source areas are the most affected. Many models were developed to describe the contaminants dispersion process in low wind conditions. Sagendorf and Dickson (1974) applied a Gaussian model and divided each computational period in ranges of 2 minutes and added the results to determine the total concentration. Brusasca *et al*. (1992) used a lagrangian particle model considering the wind meandering phenomenon. Degrazia *et al*. (2000) presented expressions to the lagrangian length scale, decorrelation time scale and eddy diffusivities in all elevations and stability conditions, furthermore, applied these expressions to a lagrangian particle dispersion model (LAMBDA) considering the database of the classic Copenhagen experiment.

Oettl *et al*. (2001) simulated the pollutant concentration on the ground level in low wind conditions, utilizing a lagrangian dispersion model. Moreira *et al*. (2005) obtained the solution of the advection-diffusion equation in low wind and stationary conditions applying the Laplace transform technique and considering the PBL as a system of multiple layers (ADMM model) (Moreira *et al*. 2006). Buske *et al*. (2007) presented an Eulerian model where the problem was analytically solved by the GILTT (Generalized Integral Laplace Transform Technique) method, considering a Gaussian in the lateral dispersion direction (Moreira *et al*., 2009). In the present search, the contaminant dispersion modeling in low wind conditions is presented in terms of the longitudinal diffusion that cannot be neglected in such situations (Buske *et al*., 2007). The stationary three-dimensional advection-diffusion equation is solved by the 3D-GILTT (Three-Dimensional Generalized Integral Laplace Transform Technique) technique (Buske *et al*., 2011). The model employs two approaches to the eddy diffusivities, an integral and other algebraic (Degrazia *et al*., 1996). The performance of this model was done considering the database of the Prairie Grass experiment accomplished in low wind (u<2 m/s) and stable conditions (Barad, 1958; Haugen, 1959).

MATERIALS AND METHODS

The atmospheric advection-diffusion can be modeled, applying the mass conservation equation. Utilizing the Reynolds decomposition rules and using gradient transport hypothesis (theory K), is obtained the parameterized advection-diffusion equation (Blackadar, 1957)

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

The terms on the left side of the equation (1) represent the advective transport and the terms on the right side represent the turbulent diffusivity, $\bar{c}$ is the mean concentration, $\bar{u}$, $\bar{v}$ and $\bar{w}$ are the wind components in x, y and z directions, respectively, and K_x, K_y and K_z are the eddy diffusivities also in x, y and z directions, respectively.

The boundary conditions to the equation (1) are

$$K_x\frac{\partial\bar{c}(L_x,y,z)}{\partial x}=K_y\frac{\partial\bar{c}(x,0,z)}{\partial y}=K_y\frac{\partial\bar{c}(x,L_y,z)}{\partial y}=K_z\frac{\partial\bar{c}(x,y,0)}{\partial z}=K_z\frac{\partial\bar{c}(x,y,\ \ )}{\partial z}=0 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(2)$$

and the source condition is given as

$$\bar{u}\bar{c}(0,y,z)=Q\delta(y \quad y_0)\delta(z \quad H_s)$$

where Q is the source emission rate (g/s), is the PBL height (m), H_s the source height (m), L_x and L_y are the limits far from the source (m) in the x and y directions, respectively, and δ is the Dirac delta function.

Assuming that the wind component $\bar{w}$ as equal to zero and the eddy diffusivity K_y has only dependency in the z direction$\left(K_y^{'}=0\right)$, the following equation is obtained

$$\bar{u}\frac{\partial\bar{c}}{\partial x} \quad \bar{v}\frac{\partial\bar{c}}{\partial y}+\frac{\partial}{\partial x}\left(K_x\frac{\partial\bar{c}}{\partial x}\right)+K_y\frac{\partial^2\bar{c}}{\partial y^2}+\frac{\partial}{\partial z}\left(K_z\frac{\partial\bar{c}}{\partial z}\right)=0 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3)$$

Therefore, the equation (3) is solved by the combination of the Laplace transform techniques and GILTT (Buske *et al*., 2007; Moreira *et al*., 2009; Buske *et al*., 2012). Consider the $\bar{v}$ wind component in the PBL contaminant dispersion modeling is very important because the horizontal wind meandering phenomenon is an important physical component (Anfossi *et al*., 2005). This wind meandering phenomenon is described by considering the $\bar{u}$ and $\bar{v}$ wind component in the model. Therefore, the meandering enhanced dispersion, characterized by wind low frequency oscillations, is a relevant mechanism to describe the atmospheric contaminants concentration.

In this work was assumed that the mean wind components $\bar{u}$ and $\bar{v}$ were calculated as

$$\bar{u}=Vsin(\theta)$$
$$\bar{v}=Vcos(\theta)$$

where V is the horizontal wind speed and θ is the wind direction.

Hereby, applying the integral transform technique in the y variable, we can expand the pollutant concentration as

$$\bar{c}(x,y,z)=\sum_{n=0}^{N}\frac{\bar{c}_n(x,z)\zeta_n(y)}{N_n^{\frac{1}{2}}} \quad \ldots\ldots\ldots\ldots\ldots\ldots(4)$$

where $\left(\zeta_n(y)=\cos(\lambda_n y)\right)$ are orthogonal autofunctions and $\lambda_n=n\,\pi/L_y$ to $n=0,1,2,3,\ldots$ are eigenvectors of the Sturm-Liouville auxiliary problem. Thus, replacing the equation (4) in the equation (3) and considering $\left(\int_0^{L_y}()\Psi_m dy\right)$ we as

$$\alpha_{n,m}\bar{u}\frac{\partial\bar{c}_n}{\partial x}+\beta_{n,m}\bar{v}\bar{c}_n+\alpha_{n,m}\bar{w}\frac{\partial\bar{c}_n}{\partial z}=\alpha_{n,m}\frac{\partial}{\partial x}\left(K_x\frac{\partial\bar{c}_n}{\partial x}\right)+\alpha_{n,m}\frac{\partial}{\partial z}\left(K_z\frac{\partial\bar{c}_n}{\partial z}\right)\quad\alpha_{n,m}\lambda_n^2K_y\bar{c}_n \quad \ldots\ldots\ldots\ldots\ldots\ldots(5)$$

here $\bar{c_n} = \bar{c_n}(x, z)$. The matrixes $\alpha_{n,m}$ and $\beta_{n,m}$ are given as

$$\alpha_{n,m} = \frac{1}{N_n^{\frac{1}{2}} N_m^{\frac{1}{2}}} \int_0^{L_y} \zeta_n(y)\zeta_m(y)\, dy = \begin{cases} 0, m \neq n \\ 1, m = n \end{cases}$$

$$\beta_{n,m} = \frac{1}{N_n^{\frac{1}{2}} N_m^{\frac{1}{2}}} \int_0^{L_y} \zeta_n^{'}(y)\zeta_m(y)\, dy = \begin{cases} \frac{2n^2}{L_y(m^2 \quad n^2)}[cos(n\pi)cos(m\pi) \quad 1], m \neq n \\ 0, \qquad\qquad m = n \end{cases}$$

The concentration $\bar{c_n}(x, z)$ is written as

$$\bar{c_n}(x, z) = \sum_{i=0}^{I} \overline{c_{n,\iota}}(x)\varsigma_i(z) \qquad \text{………………………………………… (6)}$$

Replacing the equation (6) in the equation (5) and considering $\int_0^h (\,)\, \varsigma_j(z)dz$, we can written the following equation in a matrix form

$$Y^{''}(x) + F \quad Y^{'}(x) + G \quad Y(x) = 0 \qquad \text{…………………………………………. (7)}$$

where $Y(x)$ is the column vector with components $\overline{c_{n,\iota}}(x)$ and the matrices F and G are defined, respectively, as: $F = B^{-1}D$ and $G = B^{-1}E$. The matrices B, D and E are given, respectively, as

$$b_{i,j} = \alpha_{n,m} \int_0^h K_x \varsigma_i(z)\varsigma_j(z)dz$$

$$d_{i,j} = \quad \alpha_{n,m} \int_0^h \bar{u}\, \varsigma_i(z)\varsigma_j(z)dz + \alpha_{n,m} \int_0^h K_x^{'} \varsigma_i(z)\varsigma_j(z)dz$$

$$e_{i,j} = \quad \alpha_{n,m} \int_0^h \bar{w}\, \varsigma_i^{'}(z)\varsigma_j(z)dz + \alpha_{n,m} \int_0^h K_z^{'}\, \varsigma_i^{'}(z)\varsigma_j(z)dz \quad \alpha_{n,m}\lambda_i^2 \int_0^h K_z\, \varsigma_i(z)\, \varsigma_j(z)dz \quad \alpha_{n,m}\lambda_i^2 \int_0^h K_y\, \varsigma_i(z)\varsigma_j(z)dz \quad \beta_{n,m} \int_0^h \bar{v}\, \varsigma_i(z)\varsigma_j(z)dz$$

To solve the problem of the equation (7), we applying an order reduction

$$Z^{'}(x) + H \quad Z(x) = 0 \qquad \text{………………………………………….. (8)}$$

The resultant system of ordinary differential equations represented by equation (8) is analytically solved using the Laplace transform and diagonalization (Buske *et al.*, 2012).

Turbulence parameterization

The performance of the model to simulate the observed concentrations was done utilizing integral and algebraic eddy diffusivities. This is the first time that the integral approach will be considered in the present model. The integral formulation is based in the Taylor statistical diffusion theory (Degrazia *et al.*, 1996) and describes the PBL turbulence in stable conditions. Furthermore, this formulation considers the pollutant plume memory effect, modeled by the autocorrelation function in the Taylor diffusion theory. This memory effect disappears for large travel times of the contaminant plume and the fluid particles are only influenced by the local properties of the turbulence.

$$\frac{K_\alpha}{u} = \frac{0.07\sqrt{c_i}(1 \quad z/\quad)^{3/4}\, z/}{(f_m)_i^{4/3}} \int_0^\infty \frac{sin\left[\left(18.24(1 \quad z/\quad)^{3/4}X\ \right)(f_m)^{2/3}\frac{z}{h}n^{'}\right]}{(1 + n^{'5/3})n^{'}} dn^{'}$$

An approximate result to the integral approach is the algebraic approach that practically reproduces similar results (Degrazia *et al.*, 1996)

$$K_\alpha = \frac{2\sqrt{\pi}0.64u \quad a_i^2(1 \quad z/\quad)^{\alpha_1}(z/\quad)X\ \left[2\sqrt{\pi}0.64a_i^2(z/\quad) + 8a_i(f_m)_i(1 \quad z/\quad)^{\alpha_1/2}X\ \right]}{\left[2\sqrt{\pi}0.64(z/\quad) + 16a_i(f_m)_i(1 \quad z/\quad)^{\alpha_1/2}X\ \right]^2}$$

where $i = (u, v, w)$, u is the friction velocity, X is the dimensionless distance

$$X = \frac{xu}{\bar{u}}$$

is the stable boundary layer height, $\propto_1$ is an constant and

$$a_i = \frac{(2.7c_i)^{1/2}}{(f_m)_{n,i}{}^{1/3}}$$

here $c_{v,w} = 0.4$, $c_u = 0.3$ and $(f_m)_i$ is the reduced frequency of the stable spectral peak

$$(f_m)_i = (f_m)_{n,i}\left(1 + 3.7\frac{z}{\Lambda}\right)$$

where, $(f_m)_{n,i}$ is the frequency of the spectral peak in the surface for neutral conditions $\left[(f_m)_{n,w} = 0.33;\ (f_m)_{n,v} = 0.16;\ (f_m)_{n,u} = 0.045\right]$, z is the height above the ground and Λ is the local Monin-Obukhov length described as

$$\Lambda = L\left(1 \quad \frac{z}{}\right)^{5/4}$$

Wind profiles

The wind is parameterized by power and similarity law (Panofsky and Dutton, 1984). The wind power law is described as

$$\frac{\bar{V}}{\bar{V_1}} = \left(\frac{z}{z_1}\right)^{\alpha}$$

where $\bar{V}$ and $\bar{V_1}$ are the horizontal mean wind speeds in the z and z_1 heights. The wind similarity law can be described as

$$\bar{V} = \frac{u}{k}\left[ln\left(\frac{z}{z_0}\right) \quad \psi_m\left(\frac{z}{L}\right)\right] \quad fo \;\; z \le z_b$$

and

$$\bar{V} = \bar{V}(z_b) \quad for \;\; z > z_b$$

here $z_b = min[|L|; 0.1 \quad]$, $k \approx 0.4$ is the von-Kármán constant and z_0 is the terrain roughness. The stability function ψ_m is given in terms of the Businger relationship

$$\psi_m\left(\frac{z}{L}\right) = \quad 4.7\frac{z}{L}$$

Experimental data

To validate the model in low wind ($\bar{V} < 2\,m/s$) and stable conditions, data reported in the classic Prairie Grass experiment was utilized (Cramer *et al.*, 2017). This low wind information never was utilized until the moment on the present model. The height of release of the sulfur dioxide trace was of 0.5 m. The receiver height was 1.5 m. The samplers were placed in arcs of 50, 100, 200, 400 and 800 m. The wind reference height is of 2 m. The friction velocity u was calculated with base in the following expression

$$u \; = \frac{0.4\bar{u}(z_r)}{ln(z_r/z_0)}$$

The Monin-Obukhov (L) lenght was obtained following the methodology proposed by Zannetti, (1990)

$$L = 1100u^2$$

The stable planetary boundary layer height was calculated utilizing the formulation proposed by Zilitinkevith, (1972)

$$= 0.4\left(\frac{u \; L}{f_c}\right)^{1/2}$$

RESULTS AND DISCUSSION

The Figures 1 and 2 and Table 1 showed the results considering the $\bar{v}$ component as equal to zero in the equation 3. The Figure 1 shows the scatter diagram of the observed and simulated concentrations using integral eddy diffusivities and wind power and similarity law, respectively. Good results are obtained with any parameterization to the wind profile.

The Figure 2 shows the scatter diagram of the observed and simulated concentrations using algebraic eddy diffusivities and wind power and similarity law, respectively. Good results are obtained with any parameterization to the eddy diffusivities, showing the good performance of the present model to simulate the observed concentrations.

In the Table 1 is listed the statistical performance of the model (Hanna, 1989), the simulated concentrations are in agreement with the observed concentrations. The Correlation Coefficient (COR) and Factor of Two (FA2) are near to one, and the Normalized Mean Square Error (NMSE), Fractional Bias (FB) and Fractional Standard deviation (FS) are near to zero, indicating a good performance of the model. Similar results are obtained when wind power and similarity law and integral and algebraic eddy diffusivities are used. Better results to COR and FA2 are obtained when we use the integral approach to parameterize the turbulence.

Table 1. Statistical performance of the present model

Integral	NMSE	COR	FA2	FB	FS
Wind power law	0.26	0.96	0.90	-0.19	-0.41
Wind similarity law	0.36	0.97	0.95	-0.33	-0.47
Algebraic	NMSE	COR	FA2	FB	FS
Wind power law	0.25	0.89	0.85	-0.08	-0.24
Wind similarity law	0.26	0.93	0.85	-0.09	-0.35

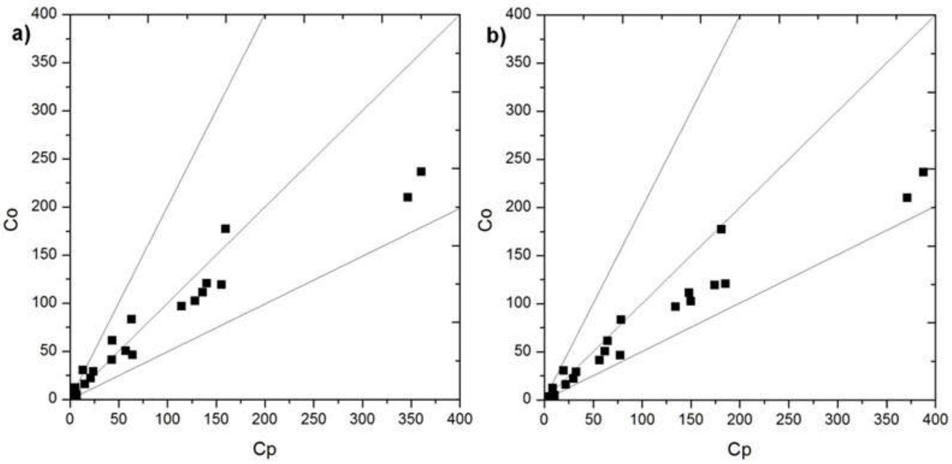

Figure 1. Scatter diagram of the observed (c_o) and simulated (c_p) concentrations using integral eddy diffusivities with a) wind power law and b) wind similarity law

Now, the Figures 3 and 4 and Table 2 showed the results considering the $\bar{v}$ component in the equation 3. The Figure 3 shows the scatter diagram of the observed and simulated concentrations using integral eddy diffusivities and wind power and similarity law, respectively. Better results are obtained when we compared the results with the Figure 1.

Table 2. Statistical performance of the model considering the $\bar{v}$ wind component in the equation 3

Integral	NMSE	COR	FA2	FB	FS
Wind power law	0.04	0.97	0.95	0.02	0.01
Wind similarity law	0.07	0.97	0.95	0.09	0.15
Algebraic	NMSE	COR	FA2	FB	FS
Wind power law	0.10	0.93	0.85	0.05	0.10
Wind similarity law	0.11	0.96	0.95	0.17	0.15

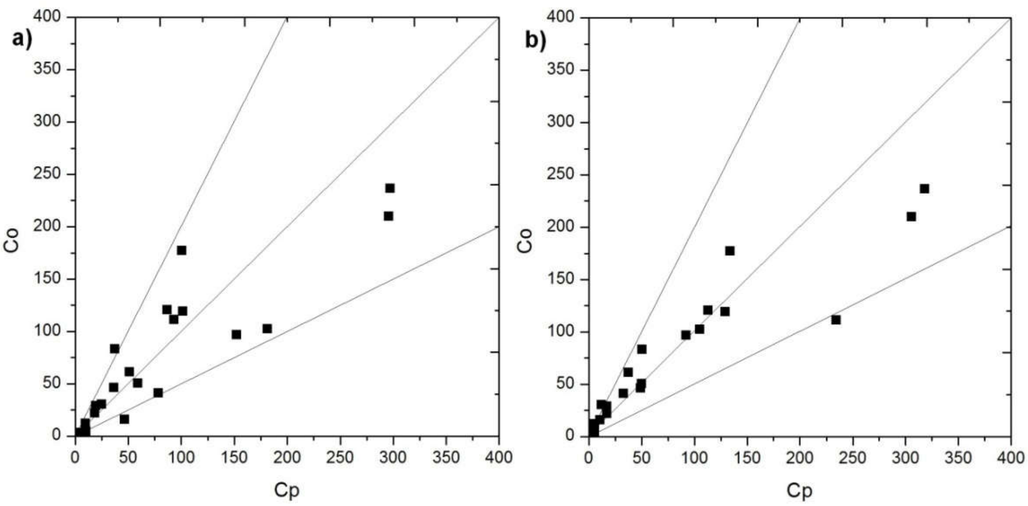

Figure 2. Scatter diagram of the observed (c_o) and simulated (c_p) concentrations using algebraic eddy diffusivities with a) wind power law and b) wind similarity law

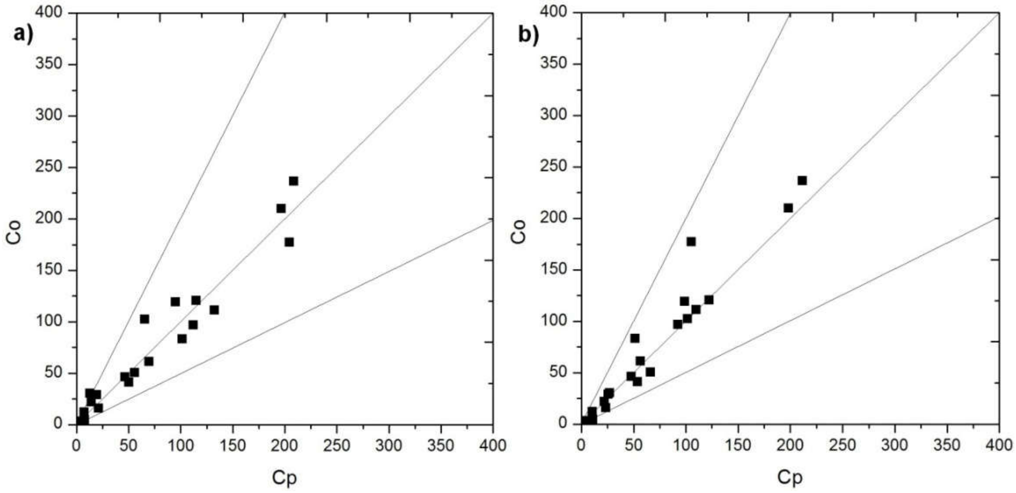

Figure 3. Scatter diagram of the observed (c_o) and simulated (c_p) concentrations using integral eddy diffusivities considering the $\bar{v}$ wind component, with a) wind power law and b) wind similarity law

The Figure 4 shows the scatter diagram of the observed and simulated concentrations using algebraic eddy diffusivities and wind power and similarity law, respectively, considering the $\bar{v}$ component in the equation 3. Better results are obtained when we compared the results with the Figure 2. In the Table 2 is listed the statistical performance of the model (Hanna, 1989) considering the $\bar{v}$ component in the equation 3. Here, better results are obtained comparing with the performance listed in the Table 1. The COR and FA2 are near to one and the NMSE, FB and FS are near to zero. Better results are obtained when we use the integral approach to parameterize the turbulence.

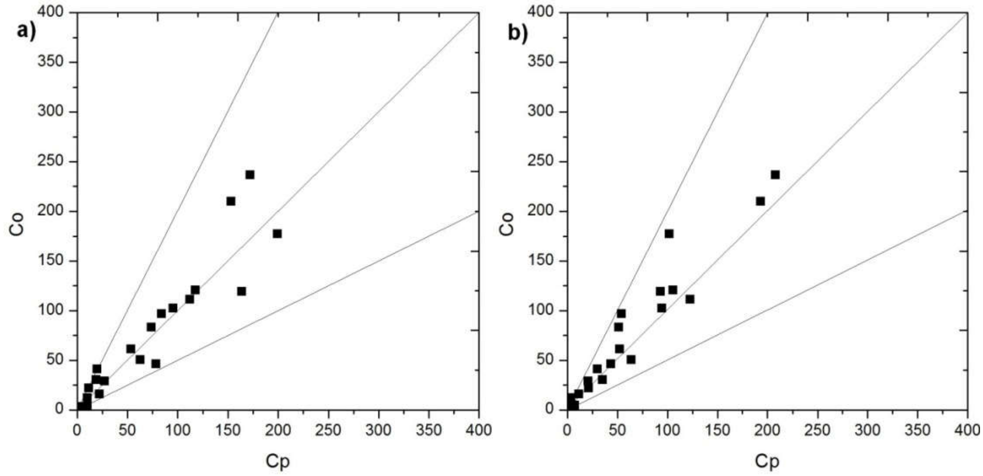

Figure 4. Scatter diagram of the observed (c_o) and simulated (c_p) concentrations using algebraic eddy diffusivities considering the $\bar{v}$ wind component, with a) wind power law and b) wind similarity law

Therefore, the simulations that consider both $\bar{u}$ and $\bar{v}$ wind components show better results, indicating the importance of the present study.

Conclusions

The choice of the turbulent parameterization in the air pollution models has an important contribution in the calculation of the contaminant concentration in the PBL. Furthermore, the turbulent parameterization describe the diffusion and transport processes observed in the low atmosphere. The performance of each model depends on the way with that the turbulent parameters are related with the evolution of the turbulent patterns of the PBL. Two turbulent parameterizations in a three-dimensional Eulerian model were tested in this work. The model is based in the solution of the advection-diffusion equation. The solution is obtained applying the integral transform technique. The model was tested with integral and algebraic eddy diffusivities. The wind profile was represented by wind power and similarity law.

The results of the simulation using integral and algebraic eddy diffusivities were positive when compared with the database observed in the Prairie Grass experiment. Good results are also obtained when wind power and similarity law are used to parameterize the wind profile. The statistical results exhibit a good agreement between the experimentally observed data and simulated by the present model. Better results are obtained in all simulations when we consider the $\bar{u}$ and $\bar{v}$ wind component in the model. In meandering situations, the COR and $FA2$ are more near to one and $NMSE$, FB and FS are more near to zero, indicating the better results observed in this situations.

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