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SIMULATION OF POLLUTANT DISPERSION UNDER LOW WIND CONDITIONS IN A STABLE ATMOSPHERIC BOUNDARY LAYER

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Abstract. *The present study proposes a mathematical model for dispersion of contaminants in low winds that takes into account the along-wind diffusion. The solution of the advection-diffusion equation for these conditions is obtained applying the 3D-GILTT method (Three-Dimensional Generalized Integral Laplace Transform Technique). The performance of the model was evaluated against the field experiments carried out at the Idaho National Engineering Laboratory carried out during stable conditions. The study suggests that the inclusion of the longitudinal diffusion improves the description of the turbulent transport process of atmospheric contaminants.*

Keywords: *analytical solution, low wind conditions, advection-diffusion equation, GILTT method*

1. INTRODUCTION

The importance of dispersion modeling in low wind conditions lies in the fact that such conditions occur frequently and are crucial for air pollution episodes. In such conditions, the pollutants are not able to travel far and thus the near-source areas are affected the most.

The classical approach based on conventional models, such as Gaussian puff/plume or the K-theory with suitable assumptions, are known to work reasonably well during most meteorological regimes, except for weak and variable wind conditions. The reasons for that are: the down-wind diffusion is neglected with respect to advection; the concentration is inversely proportional to wind speed; the average conditions are stationary and there is a lack of appropriate estimates of dispersion parameters in low wind conditions.

Various attempts have been made in literature to explain dispersion in the presence of low wind conditions by relaxing some of the limitations (Seinfeld and Pandis, 1997), (Arya, 1995), (Sharan and Gopalakrishnan, 2003). Several models have been developed to describe dispersion processes under low winds conditions. Sharan and Yadav (1998) used a model including stream-wise diffusion and variable eddy diffusivities. The eddy diffusivities were specified as linear functions of the downwind distance. The model of Cirillo and Poli (1992) gave almost identical results when compared with the ones of the model of Sharan and Yadav (1998) for the INEL dataset. Sagendorf and Dickson (1974) used a Gaussian model and also divided each computation period into 2-min time intervals, summing the results to determine the total concentration. The limitations of the said models arise from a built in assumptions of a homogeneous wind field and restrictions concerning the shape of the source. Brusasca *et al.* (1992) used a Lagrangian particle model to take meandering of the flow into account. Oettl *et al.* (2001), attempted to simulate ground-level concentrations in low wind conditions, utilizing a Lagrangian dispersion model with random time steps and a negative inter-correlation parameter for the horizontal wind components. More recently, Moreira *et al.* (2005), obtained the solution of the steady state 2D advection-diffusion equation for low wind conditions applying the Laplace transform, considering the PBL as a multilayer system (ADMM model) (Moreira *et al.*, 2006). Buske *et al.* (2007) proposed a steady state 2D mathematical model for dispersion of contaminants in low winds taking into account the along-wind diffusion. The solution of the advection-diffusion equation was obtained applying the GILTT (Generalized Integral Laplace Transform Technique) method. In the solutions obtained by the ADMM and GILTT methods a gaussian in the y direction was considered (Moreira *et al.*, 2009).

The present study proposes a mathematical model for dispersion of contaminants in low winds that takes into account the along-wind diffusion. The solution of the advection-diffusion equation for these conditions is obtained applying the

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3D-GILTT method (Three-Dimensional Generalized Integral Laplace Transform Technique) (Buske *et al.*, 2011). The performance of the model was evaluated against the field experiments carried out at the Idaho National Engineering Laboratory during stable conditions. The study suggests that the inclusion of the longitudinal diffusion improves the description of the turbulent transport process of atmospheric contaminants.

2. SOLUTION OF THE ADVECTION-DIFFUSION EQUATION

For a Cartesian coordinate system the advection-diffusion equation, under stationary conditions, based on the gradient transport hypothesis (or K-theory) combined with the continuity equation of mass, is written like (Seinfeld and Pandis, 1997):

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

where $\overline{c}(x,y,z)$ denotes the average concentration of a passive contaminant (g/m^3), $\overline{u}$, $\overline{v}$ and $\overline{w}$ are the mean wind (m/s) components along the axis $x(0 < x < L_x)$, $y(0 < y < L_y)$ and $z(0 < z < h)$. K_x, K_y and K_z are the Cartesian components of eddy diffusivity (m^2/s) in the x, y and z directions, respectively.

Equation (1) is subjected to the usual boundary conditions of zero flux at the boundaries:

$$\mathbf{K}\nabla\overline{c}\mid_{(0,0,0)} = \mathbf{K}\nabla\overline{c}\mid_{(L_x,L_y,h)} = 0 \quad (2)$$

and source conditions::

$$\overline{u}\,\overline{c}(0,y,z) = Q\delta(y-y_0)\delta(z-H_s) \quad (3)$$

where Q is the emission rate (g/s), h the height of the Atmospheric Boundary Layer (ABL) (m), H_s the height of the source (m), L_x and L_y are the limits in the x and y-axis and far away from the source (m) and d represents the generalized Dirac delta function.

In order to solve the problem (1), we initially apply the integral transform technique in the y variable. For such, we expand the pollutant concentration as:

$$\overline{c}(x,y,z) = \sum_{n=0}^{N}\frac{\overline{c_n}(x,z)\,\Psi_n(y)}{N_n^{\frac{1}{2}}} \quad (4)$$

where $(\Psi_n(y) = \cos(\lambda_n y))$ is a set of orthogonal eigenfunctions and $\lambda_n = n\pi/L_y$ for $n = 0,1,2,3,...$ are the respective eigenvalues, N_n is given by:

$$N_n = \int_0^{L_y}\Psi_n^2(y)dy \quad (5)$$

To determine the unknown coefficient, $\overline{c_n}(x,z)$, we began substituting Eq. (4) in Eq. (1) and then applying the operator $\frac{1}{N_m^{\frac{1}{2}}}\int_0^h(.)\Psi_m(y)dy$. This procedure leads to:

$$\begin{aligned}
&-\sum_{n=0}^{N}\frac{\overline{u}}{N_n^{\frac{1}{2}}N_m^{\frac{1}{2}}}\frac{\partial\overline{c_n}(x,z)}{\partial x}\int_0^{L_y}\Psi_n(y)\Psi_m(y)dy-\sum_{n=0}^{N}\frac{\overline{v}}{N_n^{\frac{1}{2}}N_m^{\frac{1}{2}}}\overline{c_n}(x,z)\int_0^{L_y}\Psi_n'(y)\Psi_m(y)dy-\\
&-\sum_{n=0}^{N}\frac{\overline{w}}{N_n^{\frac{1}{2}}N_m^{\frac{1}{2}}}\frac{\partial\overline{c_n}(x,z)}{\partial z}\int_0^{L_y}\Psi_n(y)\Psi_m(y)dy+\sum_{n=0}^{N}\frac{1}{N_n^{\frac{1}{2}}N_m^{\frac{1}{2}}}\overline{c_n}(x,z)\int_0^{L_y}K_y'\Psi_n'(y)\Psi_m(y)dy-\\
&-\sum_{n=0}^{N}\frac{\lambda_n^2}{N_n^{\frac{1}{2}}N_m^{\frac{1}{2}}}\overline{c_n}(x,z)\int_0^{L_y}K_y\Psi_n(y)\Psi_m(y)dy+\\
&+\sum_{n=0}^{N}\frac{1}{N_n^{\frac{1}{2}}N_m^{\frac{1}{2}}}\frac{\partial}{\partial x}\left(K_x\frac{\partial\overline{c_n}(x,z)}{\partial x}\right)\int_0^{L_y}\Psi_n(y)\Psi_m(y)dy+\\
&+\sum_{n=0}^{N}\frac{1}{N_n^{\frac{1}{2}}N_m^{\frac{1}{2}}}\frac{\partial}{\partial z}\left(K_z\frac{\partial\overline{c_n}(x,z)}{\partial z}\right)\int_0^{L_y}\Psi_n(y)\Psi_m(y)dy=0
\end{aligned} \quad (6)$$

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We specialize the application for a pollutant dispersion problem in atmospheric boundary layer, assuming that the reference system is orientated to the prevailing wind and considering that K_y has only dependence on the z-direction. After these assumptions the following set of N + 1 two-dimensional diffusion equations is obtained:

$$\overline{u}\frac{\partial\overline{c_n}(x,z)}{\partial x} - \frac{\partial}{\partial x}\left(K_x\frac{\partial\overline{c_n}(x,z)}{\partial x}\right) - \frac{\partial}{\partial z}\left(K_z\frac{\partial\overline{c_n}(x,z)}{\partial z}\right) + {\lambda_n}^2 K_y\overline{c_n}(x,z) = 0 \tag{7}$$

The analytical solution of the above two-dimensional problem is obtained by the GILTT approach Moreira *et al.* (2009). The mean feature of the GILTT method comprehends the steps: solution of an associate Sturm-Liouville problem, expansion of the pollutant concentration in a serie in terms of the attained eigenfunction, replacement of this expansion in the advection-diffusion equation and, finally, taking moments. This procedure leads to a set of second order differential ordinary equations, named the transformed equation. After an order reduction, the transformed problem is solved analytically by the application of the Laplace transform technique without any approximation along its derivation, except the round-off error.

Following the works of (Wortmann *et al.*, 2005) and (Moreira *et al.*, 2009), and taking advantage of the well known solution for the stationary problem with advection in the x direction, we pose the solution of problem (7) in the form:

$$\overline{c_n}(x,z) = \sum_{i=0}^{I}\overline{c_{n,i}}(x)\,\varsigma_i(z) \tag{8}$$

where $(\varsigma_i(z) = \cos(\gamma_i z))$ are a set of orthogonal eigenfunctions and $\gamma_i = i\pi/h$, $i = 0, 1, 2, 3, ...$ are respectively the set of eigenvalues of the associated Sturm-Liouville problem. Replacing Eq. (8) in Eq. (7) and taking moments, we get the second order matrix differential equation:

$$Y''(x) + FY'(x) + GY(x) = 0 \tag{9}$$

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

$$b_{i,j} = \int_0^h K_x\,\varsigma_i(z)\,\varsigma_j(z)dz \tag{10}$$

$$d_{i,j} = -\int_0^h \overline{u}\,\varsigma_i(z)\,\varsigma_j(z)dz + \int_0^h K'_x\,\varsigma_i(z)\,\varsigma_j(z)dz \tag{11}$$

$$e_{i,j} = \int_0^h K'_z\,\varsigma'_i(z)\,\varsigma_j(z)dz - \lambda_i^2\int_0^h K_z\,\varsigma_i(z)\,\varsigma_j(z)dz - \lambda_i^2\int_0^h K_y\,\varsigma_i(z)\,\varsigma_j(z)dz \tag{12}$$

To solve the problem of Eq. (8) we apply the order reduction and come out with the result:

$$Z'(x) + HZ(x) = 0 \tag{13}$$

where the matrix H has the block matrix form:

$$H = \begin{bmatrix} 0 & -I \\ G & F \end{bmatrix} \tag{14}$$

The transformed problem represented by the equation (12) is solved by the Laplace Transform technique and diagonalization, likewise in the work Wortmann *et al.* (2005). The solution is given by:

$$Z(x) = X.M(x).X^{-1}.Z(0) \tag{15}$$

where $M(x)$ is the diagonal matrix with elements $e^{-d_i x}$. Here X is the matrix of the eigenvectors of the matrix H and Z(0) is the initial condition vector giving by the vector $Z(0) = col[Z_1(0), Z_2(L_x)]$ where $Z_1(0) = \frac{Q}{r}\,\zeta_m(H_s)A^{-1}$ and $Z_2(L_x) = 0$. A^{-1} is the inverse of matrix $a_{n,m} = \int_0^h \overline{u}\,\zeta_n(z)\,\zeta_m(z)dz$. No approximation is made along the derivation of solution, except for the round-off in equations (4) and (8).

Once $\overline{c_n}(x,z)$ is known we are in a position to write the final three-dimensional solution of problem (1) which is given by Eq. (4). In the case that $K_x \to 0$, we obtain the solutions of Buske *et al.* (2011) and Moreira *et al.* (2009).

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3. TURBULENT PARAMETERIZATION

To represent the near-source diffusion in weak winds the eddy diffusivities should be considered as functions of not only turbulence (e.g., large eddy length and velocity scales), but also of distance from the source (Arya, 1995). Following this idea, Degrazia *et al.* (1996) proposed an algebraic formulation for the eddy diffusivities, which takes the form:

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

where $X^* = xu_*/\overline{u}h$ represents the nondimensional distance, h is the height of the turbulent Stable Boundary Layer (SBL), α_1 is a constant that depends on the evolution state of the SBL, $(f_m)_i = (f_m)_{n,i}(1+3.7\frac{z}{\Lambda})$ is the frequency of the spectral peak (i standing for the turbulent velocity components u, v and w), $(f_m)_{n,i}$ is the frequency of the spectral peak in the neutral stratification $[(f_m)_{n,w} = 0.33; (f_m)_{n,v} = 0.22; (f_m)_{n,u} = 0.045$ (Sorbjan, 1989)], z is the height above the ground, $\Lambda = L(1-z/h)^{(1.5\alpha_1-\alpha_2)}$ is the local Monin-Obukhov length $[\alpha_1 = 1.5; \alpha_2 = 1$ (Nieuwstadt, 1984)] and $a_i = (2.7c_i)^{1/2}/(f_m)_{n,i}^{1/3}$ $[c_{v,w} = 0.4; c_u = 0.3]$. More details in (Degrazia *et al.*, 1996). The generalized eddy diffusivity (15), as a function of downwind distance, is dependent on z and yields a description of turbulent dispersion in the near fields of a source.

The wind speed profile is described by a power law (Panofsky and Dutton, 1988).

4. EXPERIMENTAL DATA AND MODEL EVALUATION

The data utilized to evaluate the performance of the model are constituted by a series of diffusion tests conducted under stable conditions for surface based releases with light winds over flat, even terrain: the results are published in a U.S. National Oceanic and Atmospheric Administration (NOAA) report (Sagendorf and Dickson, 1974). Because of wind direction variability a full 360^o sampling grid was implemented. Arcs were laid out at radii of 100, 200 and 400 m from the emission point. Samplers were placed at intervals of 6^o on each arc, for a total of 180 sampling positions. The receptor height was $0.76m$. The tracer SF_6 was released at a height of $1.5m$. The $1h$ average concentrations were determined by means of an electron capture gas chromatograph. Wind measurements were provided by lightweight cup anemomenters and bivanes at the 2, 4, 8, 16, 32 and 61 m levels of the $61-m$ tower located on the $200m$ arc. Table 1 summarizes the conditions of the tests 4-14. In the table, the hourly average wind speed, u, and the standart deviation of the horizontal wind direction over the averaging period considered, σ_θ, are reported at the $2m$ level.

Table 1. Dispersion condition of the tests 4-14 for the stable case (Sagendorf and Dickson, 1974).

Run	$\overline{u}$ (2 m) (ms^{-1})	u_* (ms^{-1})	σ_θ (deg)	L (m)	h (m)
4	0,7	0,047	13,6	2,4	13
5	0,8	0,053	28,4	3,1	16
6	1,2	0,08	11,4	7,1	30
7	0,6	0,04	23,9	1,8	11
8	0,5	0,033	49,6	1,2	8
9	0,5	0,033	21,4	1,2	8
10	1,1	0,073	24,8	5,9	26
11	1,4	0,093	37,6	9,6	37
12	0,7	0,047	28,8	2,4	13
13	1,0	0,067	12,0	4,9	23
14	1,0	0,067	17,2	4,9	23

The roughness length utilized was $0.005m$ by Brusasca *et al.* (1992) and Sharan and Yadav (1998). The Monin-Obukhov lenght (L) and friction velocity (u_*) input parameters were not available for the INEL experiment but have been evaluated. Thus, the Monin-Obukhov lenght can be written from an empirical formulation (Zannetti, 1990) as:

$$L = 1100{u_*}^2 \quad (17)$$

and the friction velocity is roughly obtained by the expression:

$$u_* = k\overline{u}(z_r)/ln(z_r/z_0) \quad (18)$$

where $z_r = 2m$ (reference height) and k is the von Karman constant (≈ 0.4). To calculate h (the height of the SBL), the relation:

$$h = 0.4(u_*L/f_c)^{1/2} \quad (19)$$

was used (Zilitinkevith, 1972).

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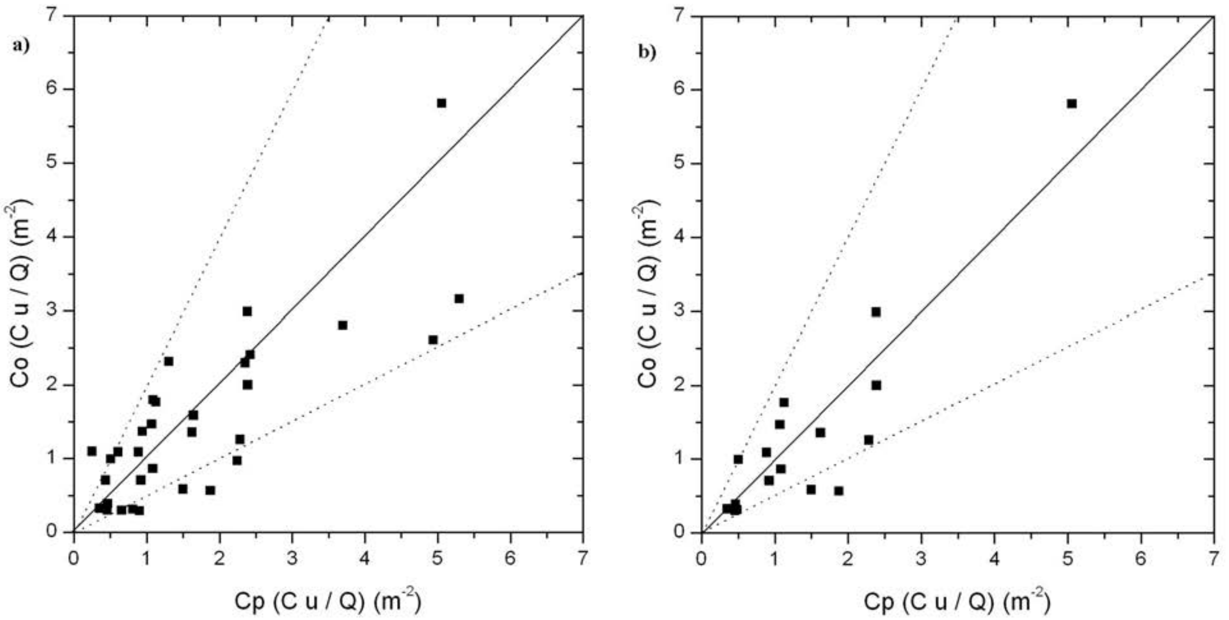

Figure 1. Observed and predicted scatter diagram of ground-level maximum crosswind concentration using the 3D-GILTT approach for: a) INEL experiment; b) INEL experiment for $u < 1m/s$. Lines indicate a factor of two.

Figure (1a) shows the observed and predicted scatter diagram of centerline concentrations (that is the centerline concentrations at the elevation of $0.76m$) using the model. Figure (1b) shows the observed and predicted scatter diagram of centerline concentrations only for $u < 1m/s$. In this case the GILTT method has been used with and without the diffusion along the wind direction outlining so the performances due to the PBL parameterization and due the capability to represent low wind scenarios.

Table 2 and Table 3 show the performance of the new model compared with other models using the statistical indices described by Hanna (1989) and defined in the following way:

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

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

FA2 (factor of 2) = $C_p/C_o \;\epsilon\; [0.5, 2]$

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

FS (fractional standard deviation) = $2(\sigma_o - \sigma_p)/(\sigma_o + \sigma_p)$

where subscripts **o** and **p** refer to observed and predicted quantities, respectively, σ is the standard deviation, **C** the concentration and the over bar indicates an averaged value. The statistical index **FB** says if the predicted quantities underestimate or overestimate the observed ones. **FA2** is the fraction of **Cp** values (normalized to 1) within a factor two of corresponding **Co** values. The statistical index **NMSE** represents the model values dispersion in respect to data dispersion. The best results are expected to have values near zero for the indices **NMSE**, **FB** and **FS**, and near one in the indices **COR** and **FA2**.

While the present approach (3D-GILTT) is based on a genuine three dimensional description an earlier analytical approach called GILTTG uses a Gaussian assumption for the horizontal transverse direction (Moreira *et al.*, 2009). The ADMM approach (Moreira *et al.*, 2005), solves the two-dimensional advection-diffusion equation by a discretisation of the ABL in a multilayer domain and also uses a Gaussian assumption for the horizontal transverse direction. The others models are based on the common Gaussian approach described in Sagendorf and Dickson (1974). In Model M-1 the stability class is determined by the average temperature gradient during the test period. Both σ_y and σ_z are determined from a single stability class using the curves from Turner (1970). The second method M-2 is the split sigma approach. In this method σ_z is determined by the temperature gradient as in the standard method, but σ_y is based on a stability class determined by the standard deviation of azimuth angle over the test period. The third procedure M-3 is similar to the standard method, except that the values of dispersion parameters are developed at the INEL. The final approach M-4 is based on the segmented plume method (Zannetti, 1990), that is a simple way to account for plume meander is to divide each test into small intervals and make separate calculations for each interval.

Analysing the statistical indices Hanna (1989) in Table 2 it is possible to notice that the model simulates satisfactorily the observed concentrations, with NMSE, FB and FS values relatively near to zero and COR and FA2 relatively near to 1. The main test of the model performance is shown in Table 3, which presents the results of the simulations considering the experiments where wind velocity is smaller than $1m/s$. We can observe that the K-model presents the better performance when considering all experiments (Table 2) and for wind speed smaller than $1m/s$ (Table 3).

Table 2. Statistical evaluation for all experiments considering others models.

Models	NMSE	COR	FA2	FB	FS
3D-GILTT	0.15	0.90	0.79	0.14	0.01
GILTTG	0.29	0.81	0.73	-0.20	-0.16
ADMM	0.25	0.79	0.79	0.02	0.08
M - 1	5.81	0.58	0.00	-1.45	-1.25
M - 2	0.60	0.71	0.70	-0.31	-0.41
M - 3	0.55	0.44	0.73	-0.04	0.17
M - 4	0.43	0.63	0.76	0.14	0.38

Table 3. Statistical evaluation considering others models only for $u < 1m/s$.

Models	NMSE	COR	FA2	FB	FS
3D-GILTT	0.09	0.96	0.94	0.03	0.08
GILTTG	0.33	0.83	0.72	-0.26	0.04
ADMM	0.21	0.85	0.92	-0.02	0.21
M - 1	6.72	0.54	0.00	-1.51	-1.15
M - 2	0.33	0.82	0.72	-0.25	-0.03
M - 3	1.02	0.21	0.56	-0.16	0.29
M - 4	0.72	0.53	0.67	0.06	0.59

5. CONCLUSIONS

A steady-state mathematical model for the dispersion of a pollutant from a continuously emitting near-ground point source in a PBL, with low wind conditions, has been described. Besides advection along the mean wind, the model takes into account the longitudinal diffusion. The closed form analytical solution of the proposed problem is obtained using the 3D-GILTT method. It is important to note that, since the influencing parameters are explicitly expressed in a mathematically closed form, the analytical solutions allow an immediate evaluation of the sensitivity of model parameters. Moreover, computer codes based on analytical expressions in general do not require prohibitive computational resources.

The present model has been evaluated in stable conditions for concentration distributions. The eddy diffusivities used in the model were derived from the local similarity and Taylor's diffusion theory. We were able to obtain a reasonable agreement between the observed concentrations and those calculated. The best results are obtained with the wind velocity smaller than $1m/s$. The present study reinforce that, the inclusion of the longitudinal diffusion and eddy diffusivities depending on the source distance, important in low wind conditions, improves the description of the turbulent transport process of atmospheric pollutants.

We focus our future attention to the task of simulating pollutant dispersion, for more realistic problem in atmosphere, considering the variable wind direction typical of low wind using the Fourier transform in the x variable.

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