SIMULATION OF THREE-DIMENSIONAL TRANSIENT POLLUTANT DISPERSION IN LOW WIND CONDITIONS USING THE 3D-GILTT TECHNIQUE

SIMULAÇÃO DA DISPERSÃO DE POLUENTES TRIDIMENSIONAL TRANSIENTE EM CONDIÇÕES DE VENTO FRACO UTILIZANDO A TÉCNICA 3D-GILTT

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Abstract: The aim of this work is to present a transient model in low wind conditions to simulate the pollutants dispersion in the atmosphere. The dispersion model is based in the advection-diffusion equation and it considers the zonal and meridional components of the wind. The transient advection-diffusion equation is solved using integral transform techniques. In this work, the generalized integral transform and Laplace techniques are used, known in the literature as GILTT and which applied to the three-dimensional problem is called 3D-GILTT (Three-dimensional Generalized Integral Laplace Transform Technique). To validate the model, data from INEL experiment (Idaho National Engineering Laboratory) carried out in the USA were used. The model simulates the observed concentrations in a satisfactory way and can be used for regulatory air quality applications.

Keywords: Pollutant dispersion. Advection-diffusion equation. Mathematical modeling

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**Resumo:** O objetivo desse trabalho é apresentar um modelo transiente em condições de vento fraco para simular a dispersão de poluentes na atmosfera. O modelo de dispersão é baseado na equação de advecção-difusão e considera as componentes zonal e meridional do vento. A equação de advecção-difusão transiente é resolvida utilizando técnicas de transformadas integrais. Neste trabalho, utilizam-se as técnicas da transformada integral generalizada e de Laplace, conhecido na literatura como GILTT e que aplicada ao problema tridimensional recebe o nome de 3D-GILTT (Three-dimensional Generalized Integral Laplace Transform Technique). Para validar o modelo foram utilizados dados do experimento INEL (Idaho National Engineering Laboratory) realizado nos EUA. O modelo simula as concentrações observadas de forma satisfatória, podendo ser utilizado para aplicações regulatórias de qualidade do ar.

**Palavras-chave:** Dispersão de poluentes. Equação de advecção-difusão. Modelagem matemática
1 INTRODUCTION

The pollutants dispersion, considering a short time range, from sources close to the surface is essentially determined by movements and processes of small scale that occur in the Planetary Boundary Layer (PBL). The physical and thermal properties of the underlying surface, together with the dynamics and thermodynamics of the lower atmosphere, determine the structure of the PBL, that is, its depth, its wind and temperature distribution, its transport, mixing and the diffusion and power dissipation properties. Variations in the depth and structure of the boundary layer occur with frequency as a result of the evolution and displacement of mesoscale and synoptic scale systems. Generally, the boundary layer becomes more slim under the influence of large scale subsidence and horizontal divergence at low levels associated with the displacement of a high pressure system (anticyclone). On the other hand, the PBL can grow to great depths and merge with deep clouds in disturbed weather conditions that are associated with low pressure systems.

Historically, the air pollution has been treated as a serious problem for large cities and shopping centers. With the advent of the industrial revolution and then with the arrival of automobiles, the air quality of most large urban and industrial areas has dropped significantly. Due to the problems caused by air pollution, it is necessary to study and understand the process of pollutants dispersion to predict the possible consequences of the environmental impact on the various ecosystems.

In the 1950s were carried out the first simultaneous measurements of concentration, plume dispersion parameters and meteorological parameters (BARAD, 1958a; BARAD, 1958b; GRYNING, 1981) in an attempt to find empirical relationships between diffusion and weather factors. Both experiments determined the concentration field on the Earth’s surface at a distance of fifty to six thousand meters from the source.

The field observations are in many time complicated by operational problems and high costs. The mathematical models are a particularly useful tool in understanding of the phenomena that control the transport, dispersion and physical-chemical transformation of pollutants immersed in the atmosphere. Therefore, the aim of this work is to evaluate the atmospheric pollutants dispersion, considering in the simulations the $u$ and $v$ wind components.
2 METHODOLOGY

The equation that models the physical phenomenon under study is the transient three-dimensional advection-diffusion equation and is given as (BLACKADAR, 1997)

\[
\frac{\partial \bar{c}}{\partial t} + \bar{u} \frac{\partial \bar{c}}{\partial x} + \bar{v} \frac{\partial \bar{c}}{\partial y} + \bar{w} \frac{\partial \bar{c}}{\partial z} = \frac{\partial}{\partial x} \left( K_x \frac{\partial \bar{c}}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial \bar{c}}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial \bar{c}}{\partial z} \right)
\]

(1)

where \( \bar{c} \) is the mean concentration, \( \bar{u}, \bar{v} \) and \( \bar{w} \) are the wind components in the \( x, y \) and \( z \) directions and \( K_x, K_y \) and \( K_z \) are the eddy diffusivities in the longitudinal, lateral and vertical directions, respectively. The terms on the left side in the equation (1) represent the advection and the terms on the right side represent the diffusion. The equation (1) is subject to zero flow conditions at \( x = 0, L_x; y = 0, L_y \) and \( z = 0, h \), zero initial condition at \( t = 0 \) and source condition given by \( \bar{u} \bar{c}(0, y, z, t) = Q \delta(y - y_0) \delta(z - H_s) \), where \( Q \) is the source emission rate \( (g/s) \), \( h \) 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 \( \delta \) is the Dirac delta function.

The \( \bar{u} \) and \( \bar{v} \) mean wind components were calculated as

\[
\bar{u} = V sen(\theta) \quad \bar{v} = V cos(\theta)
\]

(2)

in which \( V \) is the wind speed and \( \theta \) is the wind direction.

In this work it is assumed that the \( \bar{w} \) wind component is zero and that the \( K_y \) eddy diffusivity has dependence only in the direction \( z \) \( (K'_y = 0) \) (ALVES et al., 2012), thus the equation (1) is written as \( (\bar{c} = \bar{c}(x, y, z, t)) \)

\[
-\frac{\partial \bar{c}}{\partial t} - \bar{u} \frac{\partial \bar{c}}{\partial x} - \bar{v} \frac{\partial \bar{c}}{\partial y} + \frac{\partial}{\partial x} \left( K_x \frac{\partial \bar{c}}{\partial x} \right) + K_y \frac{\partial^2 \bar{c}}{\partial y^2} + \frac{\partial}{\partial z} \left( K_z \frac{\partial \bar{c}}{\partial z} \right) = 0
\]

(3)

Applying the integral transform technique to the \( y \) variable, the pollutants concentration is expanded as (BUSKE et al., 2012)

\[
\bar{c}(x, y, z, t) = \sum_{n=0}^{N} \frac{\bar{c}_n(x, z, t) \zeta_n(y)}{N_n^2}
\]

(4)

where \( \zeta_n(y) \) are orthogonal autofunctions given as \( \zeta_n(y) = \cos(\lambda_n y) \), with \( \lambda_n = \frac{n\pi}{L_y} (n = 0, 1, 2, \ldots) \), where \( \lambda_n \) o eigenvalues set and \( N_n \) is given by \( N_n = \int_0^{L_y} \zeta_n^2(y)dy \).
Replacing the equation (4) in the equation (3) and considering \( \frac{1}{N_m^2} \int_0^{L_y} \zeta_m(y)dy \) we can write

\[
\alpha_{n,m} \frac{\partial c_n(x, z, t)}{\partial t} + \alpha_{n,m} u \frac{\partial c_n(x, z, t)}{\partial x} + \beta_{n,m} v c_n(x, z, t) =
\]

\[
= \alpha_{n,m} K'_x \frac{\partial c_n(x, z, t)}{\partial x} + \alpha_{n,m} K_x \frac{\partial^2 c_n(x, z, t)}{\partial x^2} + \alpha_{n,m} K'_z \frac{\partial c_n(x, z, t)}{\partial z} +
\]

\[
+ \alpha_{n,m} K_z \frac{\partial^2 c_n(x, z, t)}{\partial z^2} - \alpha_{n,m} \lambda_n^2 K_y c_n(x, z, t)
\]

The expressions to \( \alpha_{n,m} \) and \( \beta_{n,m} \) are given as

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

(6)

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

(7)

Applying the Laplace transform technique in the equation (5) in the \( t \) variable and using the initial condition \( \{c_n(x, z, 0) = 0\} \) of the problem, we can write the following stationary problem

\[
\alpha_{n,m} r \mathcal{C}(x, z, r) + \alpha_{n,m} u \frac{\partial \mathcal{C}(x, z, r)}{\partial x} + \beta_{n,m} \mathcal{C}(x, z, r) =
\]

\[
= \alpha_{n,m} K'_x \frac{\partial \mathcal{C}(x, z, r)}{\partial x} + \alpha_{n,m} K_x \frac{\partial^2 \mathcal{C}(x, z, r)}{\partial x^2} + \alpha_{n,m} K'_z \frac{\partial \mathcal{C}(x, z, r)}{\partial z} +
\]

\[
+ \alpha_{n,m} K_z \frac{\partial^2 \mathcal{C}(x, z, r)}{\partial z^2} - \alpha_{n,m} \lambda_n^2 K_y \mathcal{C}(x, z, r)
\]

(8)

where \( \mathcal{C} \left( \mathcal{C}(x, z, r) = \mathcal{L} \{c_n(x, z, t); t \to r\} \right) \) is the Laplace transform in the \( t \) variable and \( r \) is complex.

The equation (8) is solved based in the autofunctions of the Sturm-Liouville problem and the concentration \( \mathcal{C}(x, z, r) \) is expanded as

\[
\mathcal{C}(x, z, r) = \sum_{i=0}^{l} c_{n,i}(x, r)\zeta_i(z)
\]

(9)
where $\varsigma_i(z)$ is the orthogonal autofunctions set given as $\varsigma_i(z) = \cos(\gamma_i z)$ with $\gamma_i = \frac{i\pi}{h} (i = 0, 1, 2, ...)$, in which $\gamma_i$ is an eigenvalues set.

Replacing the equation (9) in the equation (8) the problem is solved by the Generalized Integral Laplace Transform Technique (GILTT) (BUSKE et al., 2007; MOREIRA et al., 2009; BUSKE et al., 2012; SILVEIRA, 2017). The GILTT technique combines a series expansion with an integration. In the expansion, is used a trigonometric base determined with a help of a Sturm-Liouville auxiliary problem. The resultant system from ordinary differential equations is analytically solved using the Laplace transform and diagonalization.

Finally, the concentration $c_n(x, z, t)$ is calculated by Gauss-Legendre quadrature method (STROUD; SECREST, 1996). Therefore

$$
\bar{c}_n(x, z, t) = \sum_{k=1}^{M} \frac{P_k}{t} A_k C \left( x, z, \frac{P_k}{t} \right) = \sum_{k=1}^{M} \frac{P_k}{t} A_k \sum_{i=0}^{I} \varsigma_{n,i} \left( x, \frac{P_k}{t} \right) \varsigma_i(z)
$$

where $I$ is the term numbers of the sum of the inverse formula of GILTT, $A_k$, $P_k$ e $M$ are, respectively, the weights, the roots and the order of the considered quadrature and are tabulated in Stroud and Secrest book (STROUD; SECREST, 1996). Finally, replacing the problem solution 2D [equation (10)] in the equation (4), is obtained the 3D-GILTT solution of the advection-diffusion equation

### 2.1 Turbulence Parameterization and Wind Profile

To represent the turbulent diffusion close to the source in low wind conditions, the eddy diffusivities must be considered as functions not only of turbulence (length of the large eddies and the speed scale), but also from the source distance (ARYA, 1995). Therefore, (DEGRAZIA; VILHENA; MORAES, 1996) proposed the following algebraic formulation for the eddy diffusivities ($K_\alpha$, $\alpha = x, y, z$) in stable conditions, take into account the memory effect of the pollutant plume, that is, the eddy diffusivities are parameterized considering the source distance.

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

where $u_*$ is the friction velocity, $z$ is the height above the ground, $h$ is the Stable Boundary Layer (SBL) height, $a_i = (2, 7c_i)^{1/2}/(f_m)_n^{1/3}$, $i = u, v, w$, $c_u = 0.3$, $c_v, w = 0.4$, $\alpha_1 = 1.5$ is a constant which depends on the evolution of SBL, $(f_m)_n,i$ is the frequency of the spectral peak in the surface for neutral conditions $[(f_m)_n,u = 0.045; (f_m)_n,v = 0.16; (f_m)_n,w = 0.33]$, $X^*$ is the dimensionless distance given by the equation $X^* = x u_*/(\pi h)$, in which $x$ is the source
distance and \( \pi \) the mean wind speed. Finally, \((f_m)_i = (f_m)_{n,i} (1 + 0.03 a_i f_c z/u_* + 3.7 z/\Lambda)\) is the reduced frequency of the stable spectral peak, in which \(a_u = 3889, a_v = 1094, a_w = 500, f_c = 10^{-4} \text{s}^{-1}\) is the Coriolis parameter and \(\Lambda\) is the local Monin-Obukhov length described as \(\Lambda = L (1 - z/h)^{5/4}\), where \(L\) is the Monin-Obukhov length.

The following eddy diffusivities were also considered, which also take into account the memory effect of the pollutant plume (SORBJAN, 1989)

\[
K_\alpha = \frac{\sigma^2_t t}{(1 + \frac{t}{T_{Li}})^2} \left(1 + \frac{t}{4T_{Li}}\right)
\]

where \(t = x/\pi\) is the time, \(T_{Li} = \frac{z}{k} \{b_i [1 + 4.7 (z/L)] (1 - z/h) u_*\}\) is the decorrelation time scale and \(\sigma^2_t = b_i (1 - z/h)^2 u_*^2\) are the variances in the \(x, y\) and \(z\) directions, respectively, where \(b_u = 6.0, b_v = 3.3\) and \(b_w = 2.5\) and \(k\) is the von-Kármán constant \((\approx 0.4)\).

The wind is parameterized by power law (PANOFSKY; DUTTON, 1984)

\[
\frac{V}{V_1} = \left(\frac{z}{z_1}\right)^\alpha
\]

where \(V\) and \(V_1\) are the horizontal mean wind speeds in the \(z\) e \(z_1\) heights and \(\alpha\) is a constant, in which in this work the value used was \(\alpha = 0.2\).

2.2 Experimental Data

To validate the model under stable atmospheric conditions data reported in the classic INEL (USA) experiment was utilized (SAGENDORF; DICKSON, 1974). The INEL experiment consists of a diffusive tests series conducted on a flat and uniform ground. The pollutant \(SF_6\) was collected in arcs distributed \(100, 200\) e \(400\) m radius from the emission point in the \(0.76\) m height above the ground. The pollutant was released of \(1.5\) m height above the level ground. The wind in \(2\) m was obtained of the experiment. The surface roughness was \(0.005\) m.

The parameters, Monin-Obukhov length, friction velocity and PBL height were not measured in the INEL (USA) experiment, but were calculated by empirical formulations. The Monin-Obukhov length was calculated (ZANNETTI, 1990) by the expression \(L = 1100u_*^2\). The friction velocity was calculated as \(u_* = k \pi (z_r) / \ln (z_r/z_0)\), where \(z_r = 2\) m (reference height) and \(z_0 = 0.005\). The height \(h\) was calculated by the following expression (ZILITINKEVICH, 1972) \(h = 0.4(u_* L/f_c)^{1/2}\).

The meteorological parameters of the INEL experiment (SAGENDORF; DICKSON,
1974) are shown in the Table 1.

Table 1: Observed and predicted meteorological parameters through INEL experiment.

| Test | $\bar{u} \ (2 \text{ m}) \ (ms^{-1})$ | $u_\ast \ (ms^{-1})$ | $L \ (m)$ | $h \ (m)$ |
|------|--------------------------------|-----------------------|----------|---------|
| 4    | 0.7                           | 0.047                 | 2.4      | 13      |
| 5    | 0.8                           | 0.053                 | 3.1      | 16      |
| 6    | 1.2                           | 0.08                  | 7.1      | 30      |
| 7    | 0.6                           | 0.04                  | 1.8      | 11      |
| 8    | 0.5                           | 0.033                 | 1.2      | 8       |
| 9    | 0.5                           | 0.033                 | 1.2      | 8       |
| 10   | 1.1                           | 0.073                 | 5.9      | 26      |
| 11   | 1.4                           | 0.093                 | 9.6      | 37      |
| 12   | 0.7                           | 0.047                 | 2.4      | 13      |
| 13   | 1.0                           | 0.067                 | 4.9      | 23      |
| 14   | 1.0                           | 0.067                 | 4.9      | 23      |

3 RESULTS

To validate the model were used the traditional statistics indexes described by Hanna (HANNA, 1989). Were evaluated the statistics indexes, Normalized Mean Square Error (NMSE), Correlation Coefficient (COR), Factor of Two (FAT2), Fractional Bias (FB) and Fractional Standard deviation (FS). The tables 2 and 3 show the statistics results (HANNA, 1989) of the present model, considering eddy diffusivities proposed by Degrazia (DEGRAZIA; VILHENA; MORAES, 1996) and Sorbjan (SORBJAN, 1989), respectively, for transient (simulation 1) and stationary (simulation 2) cases, considering the $v$ wind component and for the transient (simulation 3) and stationary (simulation 4) cases not considering the $v$ wind component inclusion. Similar results are obtained for the transient and stationary cases independent if the meridional wind speed is considered or is not considered and independent of the parameterization for the eddy diffusivities. Best results are obtained when the $v$ wind component is considered in the model for both eddy diffusivities parameterizations. This is in according with expectations, when the meridional wind speed is considered, a more realistic PBL physics is being take into account.
Table 2: Performance of the model using eddy diffusivities proposed by Degrazia (DEGRAZIA; VILHENA; MORAES, 1996) for the transient and stationary cases, considering and not considering the $v$ wind component inclusion.

| Simulation | NMSE | COR | FAT2 | FB  | FS  |
|------------|------|-----|------|-----|-----|
| 1          | 0.04 | 0.97| 1.00 | -0.01| -0.06|
| 2          | 0.04 | 0.97| 1.00 | 0.02 | -0.03|
| 3          | 0.16 | 0.93| 0.88 | -0.17| -0.23|
| 4          | 0.12 | 0.93| 0.91 | -0.07| -0.16|

Table 3: Performance of the model using eddy diffusivities proposed by Sorbjan (SORBJAN, 1989) for the transient and stationary cases, considering and not considering the $v$ wind component inclusion.

| Simulation | NMSE | COR | FAT2 | FB  | FS  |
|------------|------|-----|------|-----|-----|
| 1          | 0.12 | 0.93| 0.94 | 0.17 | 0.03|
| 2          | 0.16 | 0.92| 0.91 | 0.20 | 0.05|
| 3          | 0.21 | 0.90| 0.88 | -0.22| -0.23|
| 4          | 0.18 | 0.89| 0.91 | -0.13| -0.18|

The scatter diagram of the observed and predicted concentrations by the present model are shown in the Figs. 1-4, where the dotted lines indicate a Factor of Two (FAT2) and the solid line indicates the central trend. The Figs. 1 and 2 consider the eddy diffusivities proposed by Degrazia [equation (11)] and the Figs. 3 and 4 the eddy diffusivities proposed by Sorbjan [equation (12)]. In the Figs. 1 and 3 the meridional wind component is included in the simulations and in the Figs. 2 and 4 the meridional wind component is not included in the simulations. The transient case is show in part a of each Figure and the stationary case is show in part b of each Figure. Looking for the Figs. 1-4, it is evident that the model presents a similar performance for the transient and stationary simulations. Comparing the Figs. 2 and 4 with the Figs. 1 and 3, better results are obtained when the $v$ wind component is considered, that is, the Figs. 2 and 4 present a greater spread of the data along the central line, indicating that the model presents a lower performance when compared with the Figs. 1 and 3.

4 CONCLUSIONS

In this work, was presented a model to simulate the pollutants dispersion in the atmosphere. The model is based on the three-dimensional transient advection-diffusion equation and the 3D-GILT technique was used to obtain the problem solution. The
Figure 1: Scatter diagrams of observed and predicted concentrations considering eddy diffusivities proposed by Degrazia. a) simulation 1 and b) simulation 2.

Figure 2: Scatter diagrams of observed and predicted concentrations considering eddy diffusivities proposed by Degrazia. a) simulation 3 and b) simulation 4.

eddy diffusivities that arise along the derivation of the model were parameterized by two methodologies available in the literature and that present a good performance, since they take into account the memory effect of the pollutant plume, that is, the source distance is included in the formulations. The performance of the model was evaluated using data observed in the low wind INEL experiment carried out in the USA and the statistical indexes described by Hanna (HANNA, 1989) were used.

The pollutant plume is simulated in a satisfactory way through the modeling architecture presented in this work. Best results are obtained when the $v$ wind component is considered, independent of the methodology used to parameterize the turbulence in the PBL. Similar results are obtained for the transient and stationary simulations. This is the first time that the solution to the proposed problem is presented in the literature, using the transient 3D-GILTT method.
and considering the $v$ wind component. As future work, we will to improve the present model, eliminating the numerical inversion in the temporal variable. Furthermore, atmospheric unstable conditions will be considered to evaluate the model performance in these situations.

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