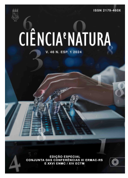
UFSM

CIÊNCIA e NATURA



ISSN 2179-460X
OPEN ACCESS

Ci. e Nat., Santa Maria, v. 46, n. spe. 1, e87264, 2024 • https://doi.org/10.5902/2179460X87624
Submitted: 03/25/2024 • Approved: 06/25/2024 • Published: 11/07/24

ERMAC e ENMC

Assessment of the pollutant dispersion, linear system and stability through the application of the 3D-GILTT method in the advection-diffusion equation

Avaliação da dispersão de poluentes, sistema linear e estabilidade através da aplicação do método 3D-GILTT na equação de advecção-difusão

Viliam Cardoso da Silveira[I], **Gustavo Braz Kurz**[I], **Daniela Buske**[I], **Régis Sperotto de Quadros**[I], **Guilherme Jahnecke Weymar**[I], **Jonas da Costa Carvalho**[I]

[I]Universidade Federal de Pelotas, Pelotas, RS, Brazil

ABSTRACT

The aim of this work is to evaluate the pollutants concentration considering a transient three-dimensional model, non-local turbulence closure and the computational time to simulate the pollutants dispersion considering different methodologies to solve the linear system that is obtained by applying the 3D-GILTT method in the three-dimensional advection-diffusion equation. To validate the model, unstable tank experiment data were considered. The results show that the Gauss-Seidel method has the shortest computational time to simulate the pollutant dispersion and the model satisfactorily simulates the observed concentrations, considering and not considering the non-local turbulence closure term.

Keywords: Advection-diffusion equation; Non-local turbulence closure; Pollutants dispersion; Analytical solution; 3D-GILTT method

RESUMO

O objetivo deste trabalho é avaliar a concentração de poluentes considerando um modelo transiente tridimensional, fechamento não local da turbulência e tempo computacional para simular a dispersão de poluentes considerando diferentes metodologias para resolver o sistema linear que é obtido pela aplicação do método 3D-GILTT na equação tridimensional de advecção-difusão. Para validar o modelo, foram considerados dados do experimento instável clássico de tanque. Os resultados mostram que o método de Gauss-Seidel possui o menor tempo computacional para simular a dispersão de poluentes e o modelo simula satisfatoriamente as concentrações observadas, considerando e não considerando o termo de fechamento não local da turbulência.

Palavras-chave: Equação de advecção-difusão; Fechamento não local da turbulência; Dispersão de poluentes; Solução analítica; Método 3D-GILTT

1 INTRODUCTION

The aim of this work is to evaluate the pollutants dispersion in the atmosphere, considering a three-dimensional transient model, the turbulence non-local closure and the 3D-GILTT method. Several studies have already been carried out using the GILTT method to solve the advection-diffusion equation, and this work is the most complete, bacause it considers dispersion in the x, y and z directions, along the time and considering turbulence non-local closure.

The application of the 3D-GILTT method to the advection-diffusion equation leads to the turbulence closure problem. The first-order closure known as gradient transport hypothesis (K-theory) is one of the most used ways to solve the advection-diffusion equation closure problem, which assumes that the turbulent flow concentration is proportional to the magnitude of the average concentration gradient. The gradient transport theory is not valid in the upper part of the convective boundary layer (CLC), because in this region there is the presence of a countergradient flow (Deardorff and Willis, 1975).

A few decades ago, it was already noticed that in the upper part of the convective boundary layer (CBL) the potential temperature flow is contrary to the potential temperature profile gradient of the medium (Deardorff, 1966). The potential temperature gradient of the medium and the flow change signs at different levels introducing a certain region into the CBL. This is in contrast to the traditional first-order turbulence closure, because it does not take into account the inhomogeneous character of the CBL turbulence. Therefore, the first-order closure equation is modified to take into account the presence of countergradient flow in the upper part of the CBL.

In order to verify the best methodology to be used in the present work, were tested different techniques to solving linear system that is generated by the 3D-GILTT technique application (LU decomposition method, iterative Jacobi method, Gauss-Seidel method and successive over-relaxation) (Burden and Faires, 2010) to reduce errors and computational time.

In this work, the advection-diffusion equation is considered in its most complete form, considering a three-dimensional model and the non-local closure term of the turbulence. To carry out the simulations, the ubuntu linux operating system was used on a notebook with core i5. The model was written in python language.

2 METHODOLOGY

Advection and diffusion atmospheric can be modeled by applying the mass conservation equation (Seinfeld and Pandis, 1997), also known as the continuity equation:

$$\frac{\partial \overline{c}}{\partial t} + \overline{u}\frac{\partial \overline{c}}{\partial x} + \overline{v}\frac{\partial \overline{c}}{\partial y} + \overline{w}\frac{\partial \overline{c}}{\partial z} = -\frac{\partial \overline{u'c'}}{\partial x} - \frac{\partial \overline{v'c'}}{\partial y} - \frac{\partial \overline{w'c'}}{\partial z} \tag{1}$$

where $\overline{c}$ $(\overline{c} = \overline{c}\,(x, y, z, t))$ denotes the average concentration of a passive contaminant, $\overline{u}$, $\overline{v}$ and $\overline{w}$ are the mean wind cartesian components (m/s) and $\overline{u'c'}$, $\overline{v'c'}$ and $\overline{w'c'}$ respectively represent the contaminant turbulent flow (g/sm^2) in the longitudinal, lateral and vertical directions.

The equation (1) presents four unknowns (turbulent flows and concentration) and therefore cannot be solved directly, leading us to the turbulence closure problem. The turbulence Fickian closure hypothesis in directions x and y is given by $\overline{u'c'} = -K_x\frac{\partial \overline{c}}{\partial x}$ and $\overline{v'c'} = -K_y\frac{\partial \overline{c}}{\partial y}$, where K_x and K_y are the eddy diffusivities (m^2/s) in the x and y directions.

In first-order closure, all the information about the turbulence complexity is contained in these eddy diffusivities. Thus, the following advection-diffusion equation (Blackadar, 1997) is obtained:

$$\frac{\partial \overline{c}}{\partial t} + \overline{u}\frac{\partial \overline{c}}{\partial x} + \overline{v}\frac{\partial \overline{c}}{\partial y} + \overline{w}\frac{\partial \overline{c}}{\partial z} = \frac{\partial}{\partial x}\left(K_x\frac{\partial \overline{c}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial \overline{c}}{\partial y}\right) - \frac{\partial \overline{w'c'}}{\partial z} \tag{2}$$

The time-dependent turbulent flow equation, as suggested by (Dop and Verver, 2001), is written as:

$$\left(1 + \beta\frac{\partial}{\partial z} + \tau\frac{\partial}{\partial t}\right)\overline{w'c'} = -K_z\frac{\partial \overline{c}}{\partial z} \tag{3}$$

where $\beta = \dfrac{S_k\sigma_w T_{l_w}}{2}$, S_k is the skewness term, σ_w the standard deviation of the vertical turbulent velocity (m/s), T_{l_w} the Lagrangian time scale (s) and τ the relaxation time (s).

Substituting the equation (3) into the equation (2) and using the Cauchy-Euler theorem, we obtain the three-dimensional time-dependent advection-diffusion equation, which considers the non-local closure of the turbulence:

$$\begin{aligned}
&\frac{\partial \overline{c}}{\partial t}+\overline{u}\frac{\partial \overline{c}}{\partial x}+\overline{v}\frac{\partial \overline{c}}{\partial y}+\overline{w}\frac{\partial \overline{c}}{\partial z}=\frac{\partial}{\partial x}\left(K_x\frac{\partial \overline{c}}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial \overline{c}}{\partial y}\right)-\frac{\partial}{\partial z}\left(\beta\frac{\partial \overline{c}}{\partial t}\right)+\\
&-\frac{\partial}{\partial z}\left(\beta\overline{u}\frac{\partial \overline{c}}{\partial x}\right)-\frac{\partial}{\partial z}\left(\beta\overline{v}\frac{\partial \overline{c}}{\partial y}\right)-\frac{\partial}{\partial z}\left(\beta\overline{w}\frac{\partial \overline{c}}{\partial z}\right)+\frac{\partial}{\partial z}\left(\beta\frac{\partial}{\partial x}\left(K_x\frac{\partial \overline{c}}{\partial x}\right)\right)+\\
&+\frac{\partial}{\partial z}\left(\beta\frac{\partial}{\partial y}\left(K_y\frac{\partial \overline{c}}{\partial y}\right)\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial \overline{c}}{\partial z}\right)-\tau\frac{\partial^2 \overline{c}}{\partial t^2}-\frac{\partial}{\partial t}\left(\tau\overline{u}\frac{\partial \overline{c}}{\partial x}\right)-\frac{\partial}{\partial t}\left(\tau\overline{v}\frac{\partial \overline{c}}{\partial y}\right)+\\
&-\frac{\partial}{\partial t}\left(\tau\overline{w}\frac{\partial \overline{c}}{\partial z}\right)+\frac{\partial}{\partial t}\left(\tau\frac{\partial}{\partial x}\left(K_x\frac{\partial \overline{c}}{\partial x}\right)\right)+\frac{\partial}{\partial t}\left(\tau\frac{\partial}{\partial y}\left(K_y\frac{\partial \overline{c}}{\partial y}\right)\right)
\end{aligned} \tag{4}$$

where K_x, K_y and K_z represent the eddy diffusivities in the longitudinal, lateral and vertical directions, respectively.

As the domain is finite, the equation (4) is subject to the following boundary and source conditions:

$$K_x\frac{\partial \overline{c}(L_x,y,z,t)}{\partial x}=K_y\frac{\partial \overline{c}(x,0,z,t)}{\partial y}=K_y\frac{\partial \overline{c}(x,L_y,z,t)}{\partial y}=K_z\frac{\partial \overline{c}(x,y,0,t)}{\partial z}=K_z\frac{\partial \overline{c}(x,y,h,t)}{\partial z}=0$$

$$\overline{u}\,\overline{c}(0,y,z,t)=Q\delta(y-y_o)\delta(z-H_s)$$

where Q is the source intensity (g/s), h is the planetary boundary layer height (m), H_s is the source height (m), L_x and L_y the limits away from the source on the x and y axis, respectively in (m) and δ is the Dirac delta function.

Applying the Laplace Transform Technique in the equation (4), to the t variable and for simplicity, we assume that the eddy diffusivity K_y has dependence only in the z direction $\left(\frac{\partial K_y}{\partial y}=0\right)$ (Alves et al., 2012), we get the following stationary problem $\left[\overline{C}=\overline{C}\,(x,y,z,r)\right]$, where $\overline{c}\,(x,y,z,0)=0$:

$$\overline{u}\frac{\partial\overline{C}}{\partial x}+\overline{v}\frac{\partial\overline{C}}{\partial y}+\overline{w}\frac{\partial\overline{C}}{\partial z}=K_x\frac{\partial^2\overline{C}}{\partial x^2}+K_x'\frac{\partial\overline{C}}{\partial x}+K_y\frac{\partial^2\overline{C}}{\partial y^2}-\beta\,r\,\frac{\partial\overline{C}}{\partial z}-(\beta\,r)'\,\overline{C}-\beta\overline{u}\frac{\partial^2\overline{C}}{\partial z\partial x}+$$

$$-(\beta\overline{u})'\,\frac{\partial\overline{C}}{\partial x}-\beta\overline{v}\frac{\partial^2\overline{C}}{\partial z\partial y}-(\beta\overline{v})'\,\frac{\partial\overline{C}}{\partial y}-\beta\overline{w}\frac{\partial^2\overline{C}}{\partial z^2}-(\beta\overline{w})'\,\frac{\partial\overline{C}}{\partial z}+\beta K_x\frac{\partial^3\overline{C}}{\partial z\partial x^2}+(\beta K_x)'\,\frac{\partial^2\overline{C}}{\partial x^2}+$$

$$+\beta K_x'\frac{\partial^2\overline{C}}{\partial z\partial x}+(\beta K_x')'\,\frac{\partial\overline{C}}{\partial x}+\beta K_y\frac{\partial^3\overline{C}}{\partial z\partial y^2}+(\beta K_y)'\,\frac{\partial^2\overline{C}}{\partial y^2}+K_z\frac{\partial^2\overline{C}}{\partial z^2}+K_z'\frac{\partial\overline{C}}{\partial z}-\tau\,r^2\,\overline{C}+$$

$$-\tau\overline{u}\,r\frac{\partial\overline{C}}{\partial x}-\tau\overline{v}\,r\frac{\partial\overline{C}}{\partial y}-\tau\overline{w}\,r\frac{\partial\overline{C}}{\partial z}+\tau\,r\,K_x\,\frac{\partial^2\overline{C}}{\partial x^2}+\tau\,r\,K_x'\,\frac{\partial\overline{C}}{\partial x}+\tau\,r\,K_y\,\frac{\partial^2\overline{C}}{\partial y^2}-r\,\overline{C}$$

where $\overline{C}$ denotes the Laplace Transform in the t variable $\overline{C}\,(x,y,z,r)=\mathcal{L}\left\{\overline{c}\,(x,y,z,t)\,;t\rightarrow r\right\}$ and r is complex.

Applying the integral transform technique to the y variable, we can expand the pollutants concentration as (Buske et al., 2012):

$$\overline{C}(x,y,z,r)=\sum_{n=0}^{N}\frac{\overline{c_n}(x,z,r)\zeta_n(y)}{N_n^{\frac{1}{2}}}$$

Using the Sturm-Liouville auxiliary problem and applying the GILTT method, the following equation can be written in matrix notation:

$$Y''(x)+F.Y'(x)+G.Y(x)=0$$

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

$$b_{i,j}=\alpha_{n,m}\int_0^h K_x\,\varsigma_i(z)\varsigma_j(z)\mathrm{d}z+\alpha_{n,m}\int_0^h\beta K_x\frac{\partial\varsigma_i(z)}{\partial z}\varsigma_j(z)\mathrm{d}z+$$

$$+\alpha_{n,m}\int_0^h(\beta K_x)'\,\varsigma_i(z)\varsigma_j(z)\mathrm{d}z+\alpha_{n,m}\int_0^h\tau\,r\,K_x\,\varsigma_i(z)\varsigma_j(z)\mathrm{d}z$$

$$r_{i,j} = -\alpha_{n,m}\int_0^h \overline{u}\,\varsigma_i(z)\varsigma_j(z)\mathrm{d}z + \alpha_{n,m}\int_0^h K'_x\,\varsigma_i(z)\varsigma_j(z)\mathrm{d}z - \alpha_{n,m}\int_0^h \beta\overline{u}\frac{\partial\varsigma_i(z)}{\partial z}\varsigma_j(z)\mathrm{d}z +$$

$$-\alpha_{n,m}\int_0^h (\beta\overline{u})'\,\varsigma_i(z)\varsigma_j(z)\mathrm{d}z + \alpha_{n,m}\int_0^h \beta K'_x\frac{\partial\varsigma_i(z)}{\partial z}\varsigma_j(z)\mathrm{d}z + \alpha_{n,m}\int_0^h (\beta K'_x)'\,\varsigma_i(z)\varsigma_j(z)\mathrm{d}z +$$

$$-\alpha_{n,m}\int_0^h \tau\,\overline{u}\,r\,\varsigma_i(z)\varsigma_j(z)\mathrm{d}z + \alpha_{n,m}\int_0^h \tau\,r\,K'_x\varsigma_i(z)\varsigma_j(z)\mathrm{d}z$$

$$s_{i,j} = -\gamma_{n,m}\int_0^h \overline{v}\,\varsigma_i(z)\varsigma_j(z)\mathrm{d}z - \alpha_{n,m}\int_0^h \overline{w}\,\frac{\partial\varsigma_i(z)}{\partial z}\varsigma_j(z)\mathrm{d}z - \alpha_{n,m}\lambda_i^2\int_0^h K_y\,\varsigma_i(z)\varsigma_j(z)\mathrm{d}z +$$

$$-\alpha_{n,m}\int_0^h \beta\,r\,\frac{\partial\varsigma_i(z)}{\partial z}\varsigma_j(z)\mathrm{d}z - \alpha_{n,m}\int_0^h (\beta\,r)'\,\varsigma_i(z)\varsigma_j(z)\mathrm{d}z - \gamma_{n,m}\int_0^h \beta\overline{v}\frac{\partial\varsigma_i(z)}{\partial z}\varsigma_j(z)\mathrm{d}z +$$

$$-\gamma_{n,m}\int_0^h (\beta\overline{v})'\,\varsigma_i(z)\varsigma_j(z)\mathrm{d}z + \alpha_{n,m}\lambda_i^2\int_0^h \beta\overline{w}\,\varsigma_i(z)\,\varsigma_j(z)\mathrm{d}z - \alpha_{n,m}\int_0^h (\beta\overline{w})'\,\frac{\partial\varsigma_i(z)}{\partial z}\varsigma_j(z)\mathrm{d}z +$$

$$-\alpha_{n,m}\lambda_i^2\int_0^h \beta K_y\frac{\partial\varsigma_i(z)}{\partial z}\varsigma_j(z)\mathrm{d}z - \alpha_{n,m}\lambda_i^2\int_0^h (\beta K_y)'\,\varsigma_i(z)\varsigma_j(z)\mathrm{d}z - \alpha_{n,m}\lambda_i^2\int_0^h K_z\varsigma_i(z)\varsigma_j(z)\mathrm{d}z +$$

$$+\alpha_{n,m}\int_0^h K'_z\frac{\partial\varsigma_i(z)}{\partial z}\varsigma_j(z)\mathrm{d}z - \alpha_{n,m}\int_0^h \tau\,r^2\,\varsigma_i(z)\varsigma_j(z)\mathrm{d}z - \gamma_{n,m}\int_0^h \tau\,\overline{v}\,r\,\varsigma_i(z)\varsigma_j(z)\mathrm{d}z +$$

$$-\alpha_{n,m}\int_0^h \tau\,\overline{w}\,r\frac{\partial\varsigma_i(z)}{\partial z}\varsigma_j(z)\mathrm{d}z - \alpha_{n,m}\lambda_i^2\int_0^h \tau\,r\,K_y\,\varsigma_i(z)\varsigma_j(z)\mathrm{d}z - \alpha_{n,m}\int_0^h r\,\varsigma_i(z)\varsigma_j(z)\mathrm{d}z$$

with

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

$$\gamma_{n,m} = \frac{1}{N_n^{\frac{1}{2}}N_m^{\frac{1}{2}}}\int_0^{L_y}\frac{\partial\zeta_n(y)}{\partial y}\zeta_m(y)dy = \begin{cases} \dfrac{2n^2}{L_y(m^2-n^2)}\left[cos(n\pi)cos(m\pi)-1\right],\ \text{m} \neq \text{n} \\ 0,\ \text{m = n} \end{cases}$$

The GILTT technique combines series expansion with integration. In the expansion, is used a trigonometric base determined with the help of an auxiliary Sturm-Liouville problem. The ordinary differential equations resulting system is analytically solved using the Laplace transform and diagonalization.

Applying an order reduction in the equation $Z'\left(x\right) + H.Z\left(x\right) = 0$, we can write

$$Z(x) = X \, . \begin{bmatrix} e^{-d_1\,x} & 0 & \dots & 0 \\ 0 & e^{-d_2\,x} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & e^{-d_n\,x} \end{bmatrix} . \, X^{-1} \, . \, Z(0)$$

where H is the block matrix $H = \begin{bmatrix} 0 & -I \\ G & F \end{bmatrix}$, with X being the eigenvector matrix and d_n the eigenvalues and $Z\left(0\right)$ is the initial condition. Defining, $\xi = X^{-1} \, . \, Z(0)$, the following linear system must be solved $X\,\xi = Z\left(0\right)$, were tested different techniques to solving this linear system.

2.1 Turbulence parameterizations and experimental data

For unstable atmospheric conditions (Degrazia et al., 2001) proposed the following formulations to the eddy diffusivities, taking into account the pollutant plume memory effect:

$$K_\alpha = \frac{0.583 w_* z_i c_i \psi^{2/3} (z/z_i)^{4/3} X^* [0.55 (z/z_i)^{2/3} + 1.03 c_i^{1/2} \psi^{1/3} (f_m^*)_i^{2/3} X^*]}{[0.55 (z/z_i)^{2/3} (f_m^*)_i^{1/3} + 2.06 c_i^{1/2} \psi^{1/3} (f_m^*)_i X^*]^2}$$

where α refers to the x, y and z directions, w_* is the convective velocity scale, z_i is the convective boundary layer height, $c_i\,(c_u = 0.3; c_{v,w} = 0.36)$ is a constant, ψ is the dissipation function given by

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

where z is the height above the ground surface, L is the Monin–Obukhov length, X^* is the dimensionless distance. The wind speed profile was described by a wind power law (Panofsky and Dutton, 1984).

To validate the model under unstable atmospheric conditions, data from the classic Tank experiment (Misra, 1982) were used. The parameters used are: Monin–Obukhov length ($L = -10$ m); convective velocity scale ($w_* = 2\,m/s$); source intensity ($Q = 10\,g/s$); font height ($H_s = 300\,m$); boundary layer height ($z = 1150\,m$) and wind speed ($V = 2.6\,m/s$).

The parameters used to evaluate the performance of the linear system are: dimensionless distance $X^* = 0.5$ and the observed dimensionless pollutant concentration is 4.90.

2.2 Statistical indexes

Statistical indexes are used to evaluate the model performance in the representation of the observed data.

The statistical indexes, Normalized Mean Square Error ($NMSE$), Correlation Coefficient (COR), Factor of 2 ($FA2$), Fractional Bias (FB) and Standard Fractional Bias (FS) are evaluated (Hanna, 1989).

3 RESULTS

As we can see from the table 1, the shortest computational time to simulate the pollutants dispersion is obtained with the iterative Gauss-Seidel method. Successive over-relaxation is the method that presents the highest computational time. As expected, the Jacobi method has a higher computational time when compared with the Gauss-Seidel method. The LU decomposition and Gauss-Seidel method presents similar simulation time.

Table 1 – Computational time to simulate the pollutants dispersion

Method	**Time**	**Concentration at ground level**
LU decomposition	15m44.006s	6.210295391310229
Jacobi	16m1.388s	6.210295391310232
Gauss-Seidel	15m41.430s	6.210295391310232
Successive over-relaxation	16m20.570s	6.210299612494771

Sourche: the authors (2024)

The pollutant dispersion problem was investigated considering the countergradient term. Micrometeorological data from the Tank experiment and eddy diffusivities proposed by Degrazia (Degrazia et al., 2001) were used. To analyze the influence of the countergradient term in the turbulent transport simulation, $S_k = 0.6$ was used (Dop and Verver, 2001).

Table 2 shows the observed (c_o) and predicted (c_p) pollutants concentration at ground level.

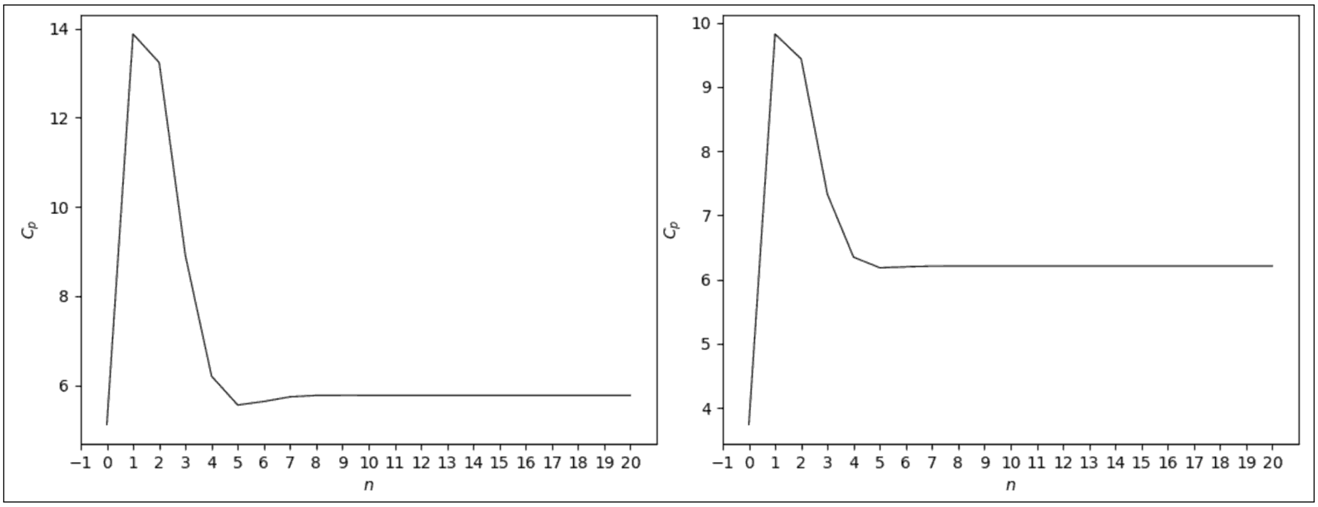
Table 2 – Observed and predicted pollutant concentration values at ground level

X^*	c_o	$c_p\,(S_k = 0)$	$c_p\,(S_k = 0.6)$
0.1	0	0.18	0.18
0.2	0.9	2.57	2.61
0.3	4.9	2.60	2.58
0.4	5.9	5.77	5.76
0.5	4.9	6.21	6.21
0.6	4.0	5.56	5.56
0.7	3.2	4.65	4.65
0.8	2.2	3.78	3.79
1.0	1.6	2.45	2.46
1.5	0.9	0.85	0.85

Source: the authors (2024)

The Figure 1 shows the solution convergence considering differents values to the dimensionless distance. For $n = 10$ the solution is stable for both cases and we used this value to evaluate the model statistical performance.

Figure 1 – Solution convergence considering $X^* = 0.4$ and $c_o = 5.9$ (figure on the left side) and $X^* = 0.5$ and $c_o = 4.9$ (figure on the right side)



Source: the authors (2024)

The statistical evaluation of the present model, considering $S_k = 0.0$ and $S_k = 0.6$ (Dop and Verver, 2001) and eddy diffusivities proposed by Degrazia (Degrazia et al., 2001) is presented in table 3.

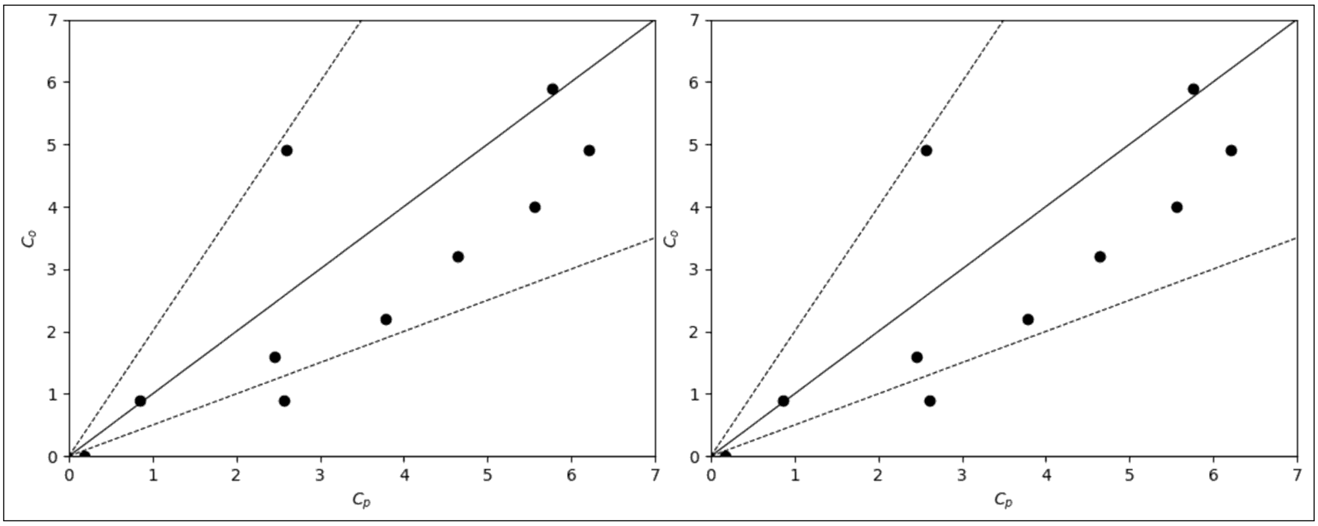
Table 3 – Model statistical performance to the Tank experiment, not considering $(S_k = 0)$ and considering $(S_k = 0.6)$ the skewness term

Simulation	$NMSE$	COR	$FAT2$	FB	FS
3D-GILTT $(S_k = 0)$	0.18	0.82	0.80	-0.19	-0.03
3D-GILTT $(S_k = 0.6)$	0.18	0.81	0.80	-0.19	-0.03
GILTTG	0.30	0.86	0.78	0.31	0.72

Source: the authors (2024)

The figure 2 shows the scattering diagram of the observed and predicted concentrations by the present model considering the skewness term, for the eddy diffusivities proposed by Degrazia (Degrazia et al., 2001).

Figure 2 – Scatter diagram of observed (c_o) and predicted (c_p) concentrations by the 3D-GILTT method to the Tank experiment and eddy diffusivities proposed by Degrazia (Degrazia et al., 2001)



For $S_k = 0.0$ (figure on the left side) and $S_k = 0.6$ (figure on the right side)
Source: the authors (2024)

Similar results are obtained considering $(S_k = 0.6)$ and not considering $(S_k = 0.0)$ the skewness term. In general, the model satisfactorily simulates the observed concentrations.

4 CONCLUSIONS

Regardless of the methodology used to solve the linear system, the pollutants concentration presents similar results and the user can decide which method to use.

The pollutants concentration is satisfactorily simulated considering the turbulence non-local closure $(S_k = 0.6)$, in comparison with results from the literature.

This solution is the most complete that was obtained using the GILTT method. In the solution, the countergradient term and longitudinal diffusion are incorporated and this model is time dependent.

The results were obtained considering $S_k = 0.6$. As future work, other values will be tested for the skewness term and other methodologies will be used to the eddy diffusivities.

ACKNOWLEDGEMENTS

The authors would like to thank CAPES for the partial financial support to carry out this work.

References

Alves, I. P., Degrazia, G. A., Buske, D., Vilhena, M. T., Moraes, O. L. L., and Acevedo, O. C. (2012). Derivation of an eddy diffusivity coefficient depending on source distance for a shear dominated planetary boundary layer. *Physica A*, 391(24):6577–6586.

Blackadar, A. K. (1997). *Turbulence and diffusion in the atmosphere: lectures in Environmental Sciences*. Springer-Verlag, Heidelberg.

Burden, R. L. and Faires, J. D. (2010). *Numerical analysis*. Brooks/Cole Cengage Learning, Canada.

Buske, D., Vilhena, M. T., 3, T. T., Quadros, R. S., and Bodmann, B. (2012). A closed form solution for pollutant dispersion in atmosphere considering nonlocal closure of the turbulent diffusion. *WIT Transactions on Ecology and The Environment*, 157:59–69.

Deardorff, J. W. (1966). The countergradient heat flux in the lower atmosphere and in the laboratory. *J. Atmos. Sci.*, 23(5):503–506.

Deardorff, J. W. and Willis, G. E. (1975). A parameterization of diffusion into the mixed layer. *J. Appl. Meteorol. Climat.*, 14(8):1451–1458.

Degrazia, G. A., Moreira, D. M., and Vilhena, M. T. (2001). Derivation of an eddy diffusivity depending on source distance for vertically inhomogeneous turbulence in a convective boundary layer. *J Appl Meteorol*, 40(7):1233–1240.

Dop, H. V. and Verver, G. (2001). Countergradient transport revisited. *J. Atmos. Sci.*, 58(15):2240–2247.

Hanna, S. R. (1989). Confidence limits for air quality model evaluations, as estimated by bootstrap and jackknife resampling methods. *Atmos. Envir.*, 23(6):1385–1395.

Misra, P. K. (1982). Dispersion of non-buoyant particles inside a convective boundary layer. *Atmos. Envir.*, 16(2):239–243.

Panofsky, H. A. and Dutton, J. A. (1984). *Atmospheric Turbulence*. John Wiley & Sons, New York.

Seinfeld, J. H. and Pandis, S. N. (1997). *Atmospheric chemistry and physics of air pollution*. John Wiley & Sons, New York.

Author contributions

1 – Viliam Cardoso da Silveira (Corresponding Author)
Meteorologist, Mathematician
https://orcid.org/0000-0001-7438-5802 • viliamcardoso2@gmail.com
Contribution: Conceptualization – Methodology – Software – Simulations – Data curation – Formal Analysis – Writing - Original draft – Preparation

2 – Gustavo Braz Kurz
Mathematician
https://orcid.org/0000-0002-8774-2394 • gustavobrk@gmail.com
Contribution: Methodology – Software – Simulations – Data curation – Formal Analysis, Writing - Review & editing

3 – Daniela Buske
Mechanical Engineer
https://orcid.org/0000-0002-4573-9787 • danielabuske@gmail.com
Contribution: Methodology – Software – Simulations – Data curation – Formal Analysis, Writing - Review & editing

4 – Régis Sperotto de Quadros
Mathematician
https://orcid.org/0000-0002-9720-8013 • quadros99@gmail.com
Contribution: Methodology – Software – Simulations – Data curation – Formal Analysis, Writing - Review & editing

5 – Guilherme Jahnecke Weymar
Mechanical Engineer
https://orcid.org/0000-0001-8216-9122 • guilhermejahnecke@gmail.com
Contribution: Methodology – Software – Simulations – Data curation – Formal Analysis, Writing - Review & editing

6 – Jonas da Costa Carvalho
Meteorologist
https://orcid.org/0000-0001-9825-2991 • jonascc@yahoo.com.br
Contribution: Methodology – Software – Simulations – Data curation – Formal Analysis, Writing - Review & editing

How to cite this article

Silveira *et al.* (2024). Assessment of the pollutant dispersion, linear system and stability through the application of the 3D-GILTT method in the advection-diffusion equation. *Ciência e Natura*, Santa Maria, v. 46, spe. 1, e87264. https://doi.org/10.5902/2179460X87624