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ANALYTICAL SOLUTION FOR CONTAMINANT DISPERSION MODEL IN RIVERS AND CANALS APPLYING THE METHOD GILTT

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ABSTRACT

In this paper we present an analytical solution for advection-diffusion equation, which models the problem of contaminant dispersion in rivers and canals. Therefore, are considered the two-dimensional vertical and three-dimensional models in steady state. The models are valid for variables velocity profiles and turbulent diffusivities. The approach for the resolution of models is the GILTT method. We also present numerical simulations.

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INTRODUCTION

In today's context of water pollution and scarcity, several research have studied the issue of pollutants dispersion in aquatic environments. Given that experimental researches are expensive and present operational problems, mathematical modeling proves a useful tool to predict the risk of contamination and impacts of pollution sources on the various ecosystems. The main models that can be used to simulate the dispersion of pollutants, are: Lagrangian, in which changes in the concentration follow the movement of the fluid, and the Eulerian, wherein the behavior of concentration is described relative to a point fixed in space (Munson, Young; Okiishi, 2004). In this work we use the Eulerian model, whose main characteristic is the solution of advection-diffusion equation. Although the numerical methods are efficient tools to solve complex problems, the analytical solutions are more advantageous because they provide a closed form solution, allowing explicitly analyze all parameters of a problem. Moreover, such solutions usually do not have the numerical dispersion problems which often occur in numerical simulations (Costa; Castro, 2005). In the literature we can find several works with analytical solutions of the advection-diffusion equation for contaminant dispersion problem in aquatic environments, but the three-dimensional analytical solutions are scarce ((Runkel, 1996); (Gandolfi; Facchi, 2001); (Dias, 2003); (Neves, 2012);(Yeh; Tsai, 1976); (Wang; McMillan; Chen, 1978); (Mazumder; Xia, 1994);(Weymar *et al*., 2010); (Barros, 2004); (Garcia, 2009)). Therefore, the objective of this paper is present numerical simulations to the dispersion of pollutants in rivers and canals for the three-dimensional advection-diffusion equation, through GILTT method.

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(*Generalized Integral Laplace Transform Technique*), following the idea of the solution presented by Buske *et al*. (2012). The GILTT technique is used to predict the behavior of the dispersed pollution, which is a spectral method that combines a series expansion with an integration. A full review of GILTT method is found in Moreira *et al*. (2009).

Mathematical model

Three-dimensional models are conceptually most appropriate for the simulation of flow, since they represent more realistically the nature events. Such models can be applied to any water body. In this model we will consider the following assumptions:

- There aren't any restrictions to the aspect ratios of the river or canal;
- The density of the pollutant is considered approximately equal to the fluid;
- The advective effect in the longitudinal direction is much larger than the diffusive in the same direction;
- The pollutant discharge rate is considered negligible compared to longitudinal velocity of the river or canal;
- The dump is done over long periods of time so that the process is reviewed on a steady state;
- The pollutant is considered likely to suffer chemical degradation;
- The river banks, surface and bottom are non-dispersive, i.e., there has any migration of contaminants through these contours;
- The velocity component in the transverse direction shall be disregarded;
- The coefficient of lateral turbulent diffusivity, ε_y, doesn't depend on the variable *y*.

Thus, the mathematical formulation of the problem is given by:

$$\bar{u}\frac{\partial \bar{c}}{\partial x} + \bar{w}\frac{\partial \bar{c}}{\partial z} = \frac{\partial}{\partial y}\left(\varepsilon_y \frac{\partial \bar{c}}{\partial y}\right) + \frac{\partial}{\partial z}\left(\varepsilon_z \frac{\partial \bar{c}}{\partial z}\right) - \lambda \bar{c}, \quad (1)$$

subjected to the following boundary conditions:

$$\frac{\partial \bar{c}}{\partial y} = 0 \ \ at \ \ y = 0, l \ \ \text{and} \ \ \frac{\partial \bar{c}}{\partial z} = 0 \ \ at \ \ z = 0, h. \quad (1a)$$

Here we replace the source term by a source condition quoted as:

$$\bar{u}\bar{c} = Q\delta(y - y_s)(z - z_s) \ \ at \ \ x = 0, \quad (1b)$$

where $\bar{c}$ represents the average concentration of contaminant (g/m³); $\bar{u}$, $\bar{w}$ represents the mean flow velocity (m/s) in the *x* and *z* directions, respectively; $\varepsilon_y, \varepsilon_z$ represents the turbulent diffusion coefficient (m²/s) in the *y* and *z* directions, respectively; λ represents the chemical degradation coefficient of the pollutant (s^{-1}); *l* is the width of the river or canal (m); *h* is the depth of the river or canal (m), *Q* is the source strength per unit area (g/sm²); δ is the Dirac delta function and y_s, z_s represents the position of the pollution source (m) in the *y* and *z* directions, respectively.

Three-dimensional analytical solution

To solve the problem (1), initially we apply the GILTT method in the *y* variable. To this end, we expand the pollutant concentration as:

$$\bar{c}(x, y, z) = \sum_{j=0}^{\infty} \bar{c}_j(x, z)\phi_j(y), \quad (2)$$

where $\phi_j(y)$ are a set of orthogonal eigenfunctions, given by $\phi_j(y) = \cos(\alpha_j y)$, and $\alpha_j = \frac{j\pi}{l}$ (*j*=0,1,2,...) are respectively the set of eigenvalues. To determine the unknown coefficient $\bar{c}_j(x, z)$ we replace the Eq. (2) in Eq. (1), apply the chain rule for the diffusion terms and taking moments, meaning applying the operator $\int_o^l (.)\phi_i(y)\, dy$, we obtain the result:

$$\sum_{j=0}^{\infty}\bar{u}\frac{\partial\bar{c}_j(x,z)}{\partial x}\int_o^l\phi_j(y)\phi_i(y)\,dy+\sum_{j=0}^{\infty}\bar{w}\frac{\partial\bar{c}_j(x,z)}{\partial z}\int_o^l\phi_j(y)\phi_i(y)\,dy-\sum_{j=0}^{\infty}\bar{c}_j(x,z)\int_o^l\varepsilon_y^{'}\phi_j^{'}(y)\phi_i(y)\,dy+$$
$$\sum_{j=0}^{\infty}\alpha_j^2\bar{c}_j(x,z)\int_o^l\varepsilon_y\phi_j(y)\phi_i(y)\,dy-\sum_{j=0}^{\infty}\frac{\partial}{\partial z}\left(\varepsilon_z\frac{\partial\bar{c}_j(x,z)}{\partial z}\right)\int_o^l\phi_j(y)\phi_i(y)\,dy+\lambda\sum_{j=0}^{\infty}\bar{c}_j(x,z)\int_o^l\phi_j(y)\phi_i(y)\,dy=0\,. \quad (3)$$

Defining the integrals appearing in the above equation like:

$$\xi_{j,i}=\int_o^l\phi_j(y)\phi_i(y)\,dy\;;\qquad\theta_{j,i}=\int_o^l\varepsilon_y^{'}\phi_j^{'}(y)\phi_i(y)\,dy;\qquad\eta_{j,i}=\int_o^l\varepsilon_y\phi_j(y)\phi_i(y)\,dy\,, \quad (4)$$

using these definitions we rewrite Eq. (3) and considering the simplifications $\theta_{j,i}=0$ *and* $\eta_{j,i}=\varepsilon_y\xi_{j,i}$, we obtain the equation:

$$\sum_{j=0}^{\infty}\left[\xi_{j,i}\bar{u}\frac{\partial\bar{c}_j(x,z)}{\partial x}+\xi_{j,i}\bar{w}\frac{\partial\bar{c}_j(x,z)}{\partial z}+\xi_{j,i}\left(\varepsilon_y\alpha_j^2+\lambda\right)\bar{c}_j(x,z)-\xi_{j,i}\frac{\partial}{\partial z}\left(\varepsilon_z\frac{\partial\bar{c}_j(x,z)}{\partial z}\right)\right]=0\,. \quad (5)$$

Truncating the series in Eq. (5) in a convenient value *J* we obtain $\bar{c}_j=(\bar{c}_0,\bar{c}_1,\bar{c}_2,...,\bar{c}_J,)$, which leads to a set of *J* + 1 two-dimensional diffusion equations:

$$\bar{u}\frac{\partial\bar{c}_j(x,z)}{\partial x}+\bar{w}\frac{\partial\bar{c}_j(x,z)}{\partial z}=\frac{\partial}{\partial z}\left(\varepsilon_z\frac{\partial\bar{c}_j(x,z)}{\partial z}\right)-\left(\varepsilon_y\alpha_j^2+\lambda\right)\bar{c}_j(x,z)\,. \quad (6)$$

Similarly the resolution of the Eq. (1), initially we apply the GILTT method in the *z* variable. Finally, we expand the pollutant concentration as:

$$\bar{c}_j(x,z)=\sum_{n=0}^{\infty}\bar{c}_n(x)\varphi_n(z)\,, \quad (7)$$

where $\varphi_n(z)$ are a set of orthogonal eigenfunctions, given by $\varphi_n(z)=\cos(\beta_n z)$, and $\beta_n=\frac{n\pi}{h}$ (*n*=0,1,2,...) are respectively the set of eigenvalues. To determine the unknown coefficient $\bar{c}_n(z)$ we replace the Eq. (7) in Eq. (6), apply the chain rule for the diffusion terms, taking moments, meaning applying the operator $\int_o^h(.)\varphi_m(z)\,dz$ and truncating the series in a value *N*, we obtain the result:

$$\sum_{n=0}^{N}\bar{c}_n^{'}(x)\int_o^h\bar{u}\,\varphi_n(z)\varphi_m(z)dz+\sum_{n=0}^{N}\bar{c}_n(x)\int_o^h\bar{w}\varphi_n^{'}(z)\varphi_m(z)dz-\sum_{n=0}^{N}\bar{c}_n(x)\int_o^h\varepsilon_z^{'}\,\varphi_n^{'}(z)\varphi_m(z)dz+$$
$$\sum_{n=0}^{N}\bar{c}_n(x)\beta_n^2\int_o^h\varepsilon_z\,\varphi_n(z)\varphi_m(z)dz+\sum_{n=0}^{N}\bar{c}_n(x)\alpha_j^2\int_o^h\varepsilon_y\varphi_n(z)\varphi_m(z)dz+\lambda\sum_{n=0}^{N}\bar{c}_n(x)\int_o^h\varphi_n(z)\varphi_m(z)dz=0\,. \quad (8)$$

Setting $E(x)$ the vector whose components are $\bar{c}_n(x)$ and *A, B* the matrices whose entries are given respectively by:

$$A=a_{n,m}=\int_o^h\bar{u}\,\varphi_n(z)\varphi_m(z)dz\;;$$
$$B=b_{n,m}=\int_o^h\bar{w}\varphi_n^{'}(z)\varphi_m(z)dz-\int_o^h\varepsilon_z^{'}\,\varphi_n^{'}(z)\varphi_m(z)dz+\beta_n^2\int_o^h\varepsilon_z\,\varphi_n(z)\varphi_m(z)dz+$$
$$\alpha_j^2\int_o^h\varepsilon_y\varphi_n(z)\varphi_m(z)dz+\lambda\int_o^h\varphi_n(z)\varphi_m(z)dz=B \quad (9)$$

Thus, the Eq. (8) can be written in matrix form:

$$E^{'}(x) + F\,E(x) = 0\,, \tag{10}$$

where $F = A^{-1}\,B$.

Similar procedure leads to the boundary condition of transformed problem (10):

$$E(0) = \bar{c}_{j,n}(0) = Q\varphi(z_s)\phi(y_s)A^{-1}\,, \tag{11}$$

where A^{-1} is the inverse of matrix *A*.

Applying the Laplace Transform in the Eq. (10):

$$sE(s) + F\,E(s) = E(0)\,, \tag{12}$$

where $E(s)$ denote the Laplace Transform of the vector $E(x)$.

The matrix *F* is decomposed in eigenvectors and eigenvalues as $F = GDG^{-1}$ where *G* is the matrix of the eigenvectors and *D* is the diagonal matrix of the eigenvalues of *F*. Then, the Eq. (12) became:

$$(sI + GDG^{-1})E(s) = E(0)\,, \tag{13}$$

where *I* is the matrix identity. After algebraic manipulation we get:

$$E(s) = G\,(sI + D)^{-1}G^{-1}E(0)\,. \tag{14}$$

Applying the Transform Inverse of Laplace the Eq. (14), finally we obtained the solution of the transformed problem given by Eq. (10):

$$E(x) = G\begin{bmatrix} e^{-d_1x} & 0 & \cdots & 0 \\ 0 & e^{-d_2x} & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & e^{-d_Nx} \end{bmatrix}G^{-1}E(0)\,, \tag{15}$$

where d_N are the eigenvalues of the matrix F.

Then, the solution of the two-dimensional problem it is given by Eq. (7):

$$\bar{c}_j(x,z) = \sum_{n=0}^{\infty}\bar{c}_n(x)\varphi_n(z)\,, \tag{16}$$

where $\varphi_n(z) = \cos(\beta_n z)$ and $\bar{c}_n(x)$ it is given by the Eq. (15).

Therefore, the final three-dimensional solution of problem (1) is given by Eq. (2):

$$\bar{c}(x,y,z) = \sum_{j=0}^{\infty}\bar{c}_j(x,z)\phi_j(y)\,, \tag{17}$$

where $\phi_j(y) = \cos(\alpha_j y)$ and $\bar{c}_j(x,z)$ it is given by the Eq. (16).

The variables considered in this model are written in dimensionless form, being defined as:

$$C = \frac{\bar{c}}{c_0};\quad X = \frac{x}{h};\quad Y = \frac{y}{l};\quad Z = \frac{z}{h};\quad U = \frac{u}{\bar{u}};\quad K_Z = \frac{\varepsilon_z}{\bar{u}h};\quad K_Y = \frac{\varepsilon_y}{\bar{u}l}\,,$$

where C is dimensionless concentration, $\bar{c}$ is the mean concentration (g/m³), c_0 is the initial concentration (g/m³), h is the depth of the river or canal (m), l is the width of the river or canal (m), u is the speed profile (m/s), $\bar{u}$ is the average velocity (m/s) and ε_y, ε_z are the coefficients of turbulent diffusion (m²/s) in the y and z directions, respectively.

RESULTS

Below we present the results for the two-dimensional vertical and three-dimensional analytical models using GILTT method. To obtain these results it used the programming language Fortran 90. All variables considered in this analysis are in dimensionless form.

Two-dimensional vertical model

In this section we present some results found for the two-dimensional vertical analytical model. These models are typically used to rivers or channels whose depth has an important role in the diffusion and mass advection process. To obtain two-dimensional equation that models the problem of dispersion, integrated laterally the Eq. (1). Applying the method GILTT the resulting equation, we obtain the two-dimensional solution which is given in Eq. (16). The two-dimensional vertical model was validated through comparison two models found in literature (Nokes; McNulty; Wood, 1984) and (Barros, 2004). The model developed by Nokes (Nokes; McNulty; Wood, 1984) simulates the dispersion of a solution containing NaCl at a canal length of 15m and a depth of 0.15m. The canal width was 0.56m and its average speed is 0.55m/s. Von Kármán's constant, κ, is 0.35 and the friction velocity, u^*, is 0.055m/s. The source of pollution is timely and is located in the dimensionless position $Z_s = 0.75$. Moreover, the model does not incorporate longitudinal variations or chemical decay terms. However, the model developed by Barros (Barros, 2004) uses the same assumptions and parameterization adopted in this work, with the difference that the solution of the problem is obtained by numerical method GITT (*Generalized Integral Transform Technique*).

The parameterizations adopted in this simulation were (Fischer *et al*., 1979):

$$U(Z) = 1 + \frac{u^*}{\bar{u}\,\kappa}\left[1 + \ln(Z)\right]; \qquad K_z(Z) = \frac{\bar{u}\,\kappa}{u^*} Z(1-Z); \qquad K_y = 0.15\frac{h u^*}{\bar{u}\, l}.$$

The graph presented in Figure 1 shows the analytical results, obtained by the method GILTT, confronted with literature results.

Through the graph we see that there is good agreement between the results. In addition, we found that the data on the concentration predicted by the model are closer to the experimental data than the results presented by (Barros, 2004). This can be explained by the fact that the GITT method presents an approximate solution to the problem of vertical dispersion, while the solution obtained by GILTT is predominantly analytical. Figure 2 shows the graphics of concentration as a function of distance X considering different source positions. We realize that, as expected, the concentration is maximal when the source is located at the near height of the initial point of release of pollutant. We found also that in the cases presented in Figs. (2a) and (2c) concentration hardly shows variations of values, indicating that the pollutant is completely mixed with the medium, while in the case of the Fig. (2b) homogenization the pollutant with the environment occurs for distances from $X = 10$.

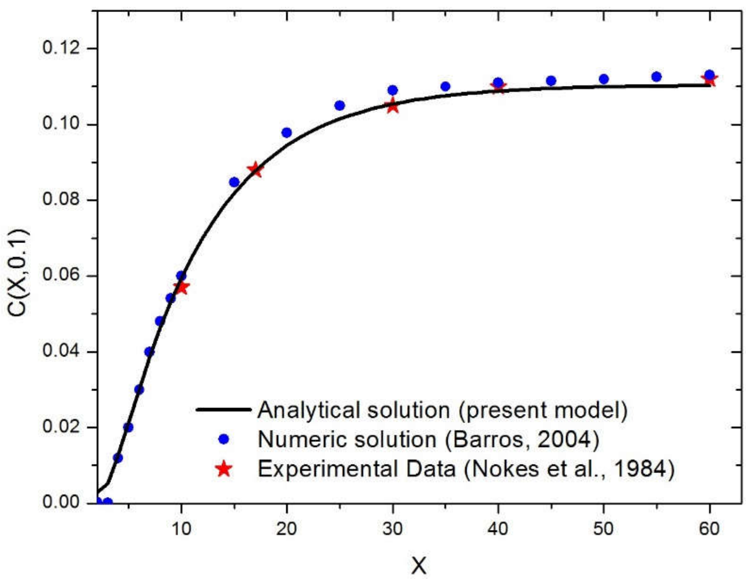

Figure 1. Validation of two-dimensional analytical model in $Z = 0.1$

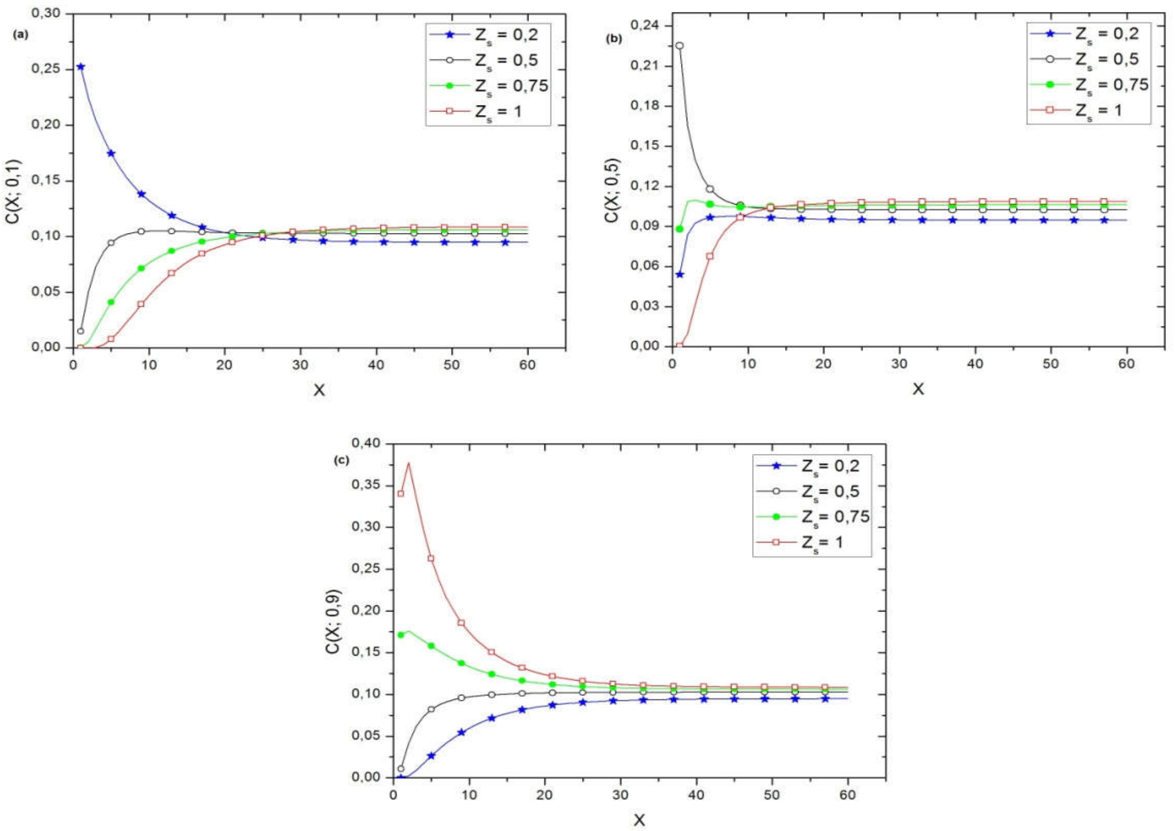

Figure 2. Pollutant concentration *C* versus distance *X* to four source positions (Z_s = 0.2; Z_s = 0.5, Z_s = 0.75, Z_s = 1) and three depths: (a) Z = 0 .1; (b) *Z* = 0.5; (c) *Z* = 0.9

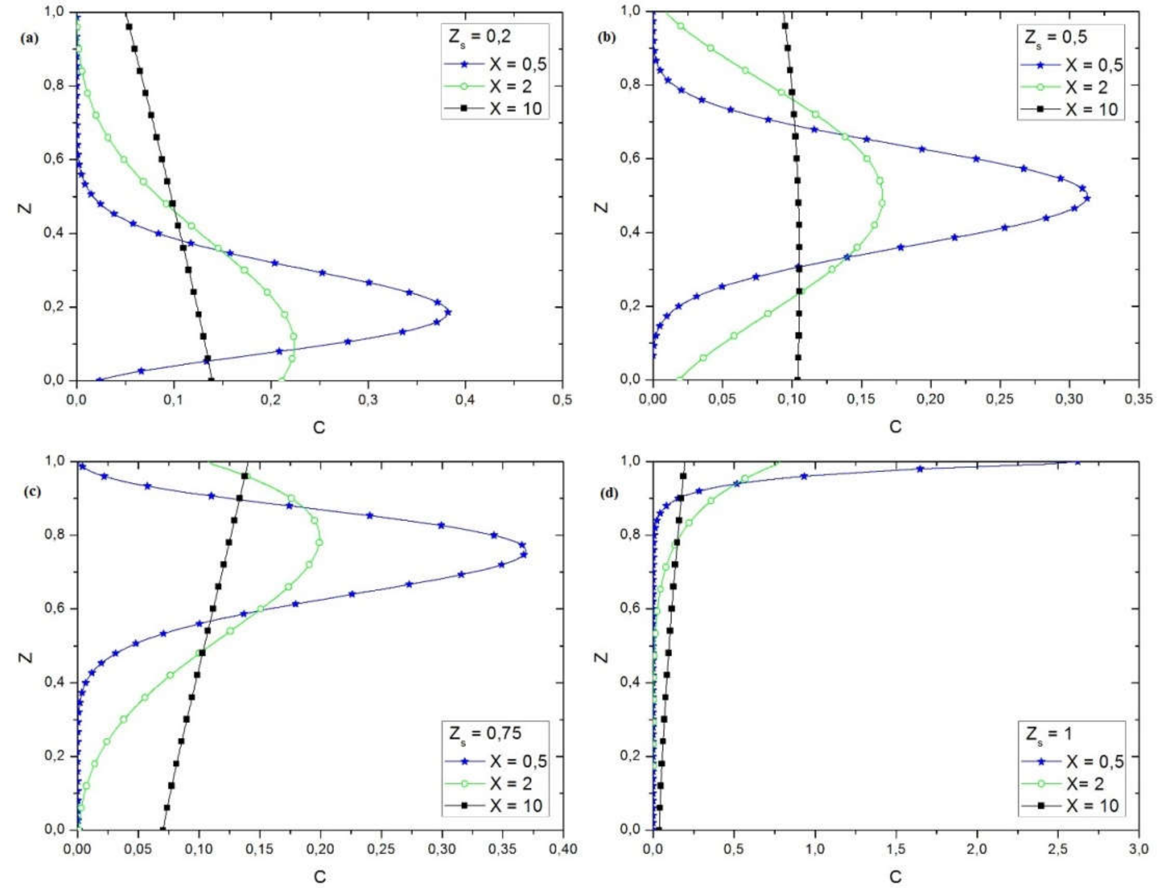

Figure 3. Vertical profile the concentration of pollutants *C* for three distances (*X* = 0.5, *X* = 2, *X* = 10) and four source positions (a) Z_s = 0.2; (b) Z_s = 0.5; (c) Z_s = 0.75; (d) Z_s = 1.

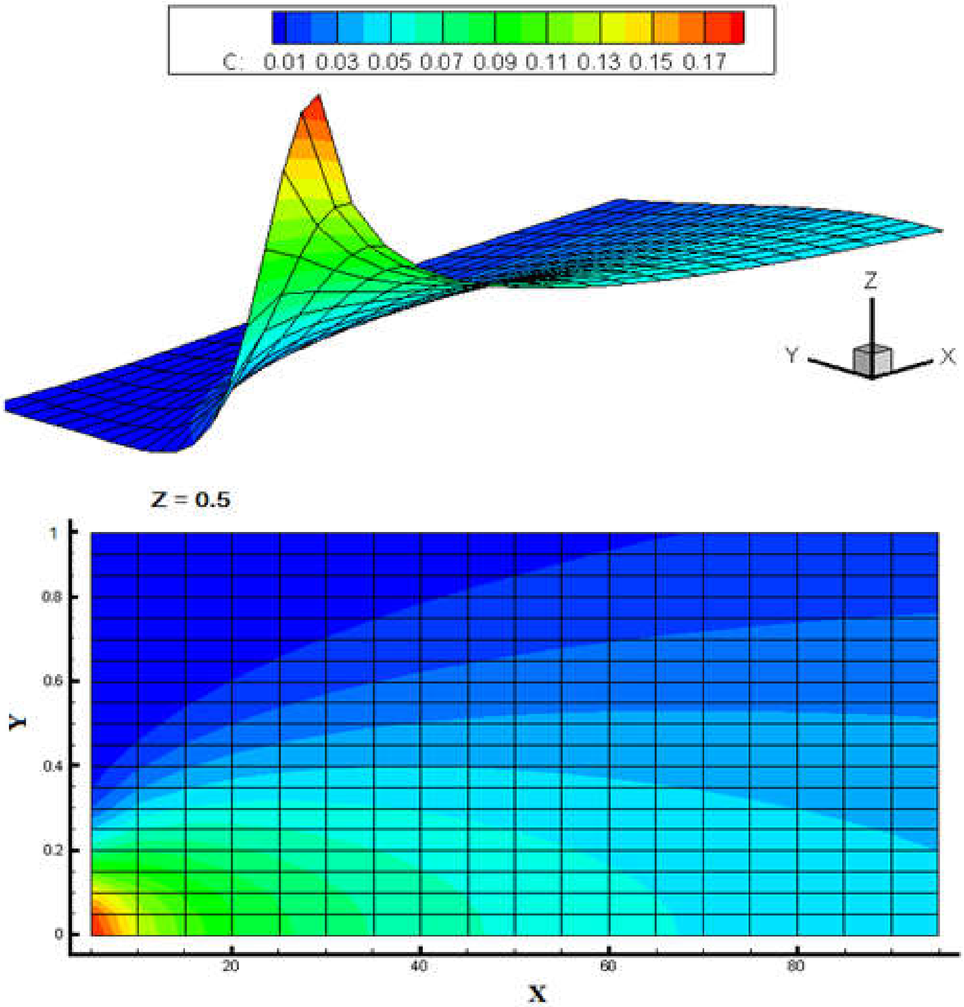

Figure 4. Behavior of the pollutant concentration *C* considering the pollution source located at the point (0; 0; 0.75)

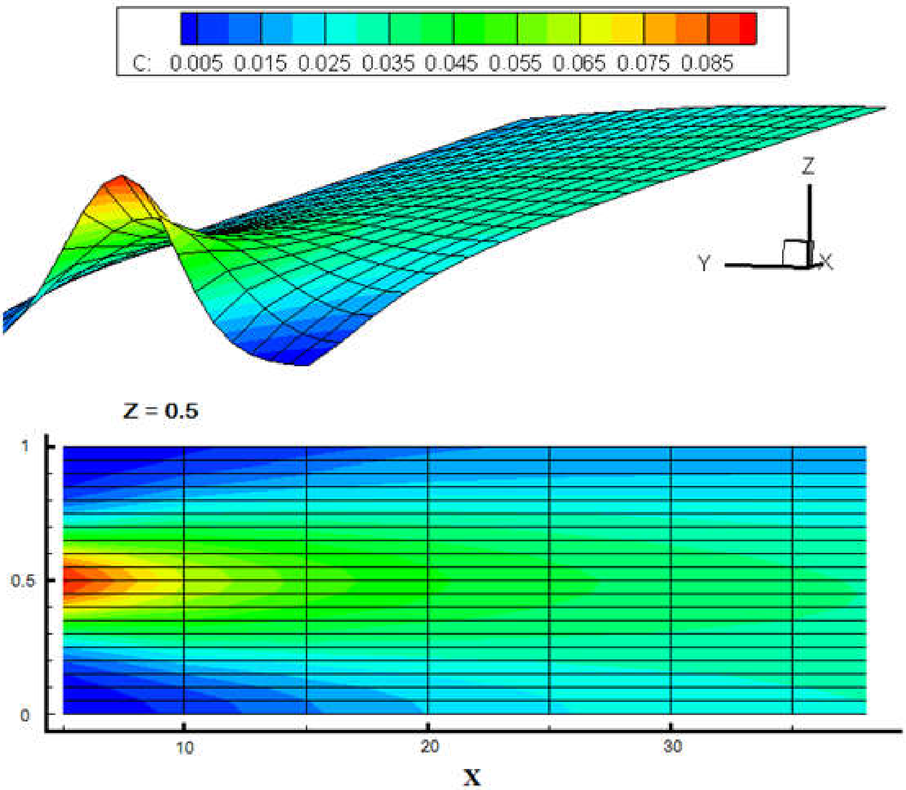

Figure 5. Behavior of the pollutant concentration *C* considering the pollution source located at the point (0; 0.5; 0.75)

Three-dimensional model

In this section we present preliminary results for the three-dimensional analytical model. For this case it was not possible to validate the model, because of the difficulty of finding experimental data in the literature. To obtain the concentration of pollutants were used the data described in Nokes, Mcnulty and Wood (1984), presented in the previous section, adding the data dimensionless $Q = 1$. Figure 3 presents the graphics of depth Z versus concentration C considering distances and different source positions. Through the graphical observed, for all font heights analyzed, the concentration reaches its maximal value at the height the polluting source is located and the concentration shows higher values for closer distances contaminant disposal site. In addition, we find that for most remote distances from the source profile concentration does not show large variations, i.e., there is a tendency to obtain a homogeneous profile concentration. The Fig. 4 shows, at different angles, the process of dispersing contaminants over a river, in which the polluting source is located at point (0; 0; 0.75). Similarly, the Fig. 5 shows the behavior of concentration of contaminants over a river, with the pollution source is located at point (0; 0.5; 0.75). As in the previous case, we note that the level of concentration is more accentuated near the release point of the pollutant and disperses quickly in the direction of flow. Also we observe that, as expected, the concentration of pollutants reaches its maximal value near the dump site and that the level of concentration decreases with increasing distance from the pollution source. Moreover, we realize that the pollutant disperses quickly in the longitudinal direction of the river, because it is influenced by the flow velocity in that direction.

Conclusion

In this paper we present an analytical solution for two-dimensional vertical and three-dimensional models in steady state, which simulates the contaminant dispersion process in rivers and canals. The models are valid for variables velocity profiles and turbulent diffusivities. We note that, for the two dimensional case studied, the analytical results obtained were compared with experimental data, that the best numerical results found in the literature. The three-dimensional model, we observed that the preliminary results were satisfactory and consistent with the physics of the problem, showing a similarity in relation to those found for the two-dimensional problem. The GILTT method has been applied with great success to model the pollutants dispersion in the atmosphere. In this paper we present an extension of this method, applied to the problem of modeling the pollutants dispersion in rivers and canals. Therefore, we conclude that the GILTT method is effective in solving the problem studied, showing that this technique is also promising in aquatic environments. For future work, we intend to improve the three-dimensional model studied and search the literature data to compare with the results obtained.

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