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CONTAMINANT DISPERSION MODEL IN A WATER BODY - CASE STUDY: RIO PARAIBUNA

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1. INTRODUCTION

Water pollution is one of the most debated issues among environmentalists; many national and international conferences focus on presenting ways to prevent and control the problem. Studies of this problem have grown a lot, due to the fact that more and more rivers and channels have been contaminated due to sewage dumping, discharge of industrial waste treated improperly, releases of solid and toxic waste, among others (AGÊNCIA NACIONAL DAS ÁGUAS, 2019).

This concern with the pollution of our waters and with the ecosystem as a whole, encourages the creation of alternative research that allows the control and evaluation of the dispersion of pollution and risks in the environment, aiming at the good use of natural resources.

In order to anticipate and avoid critical pollution events, it is essential to know the processes that govern the transport of pollutants in the aquatic environment. According to Ramos *et al.* (2014), mathematical models are indispensable technical instruments that assist in environmental management and safety.

In this scenario of great environmental concern, mathematical modeling presents itself as a resource that has been increasingly used and explored in studies of ecosystems, as it shows high scientific value and usefulness in the prognosis and assessment of environmental impacts.

Mathematical models are tools that aim to represent a real system through mathematical functions. Most models are simplifications of a real problem, but these must take into account the essential characteristics of the problem (Moreira *et al.*, 2005). One of the most used dispersion models for environmental monitoring is the Gaussian model, but this has certain limitations in its attempt to represent reality. It should be noted that this model is widely used in both air and water monitoring agencies, due to its simplicity (Ramos *et al.*, 2014). The concentration field in this model follows a Gaussian distribution, that is, it is homogeneous, but not isotropic. These models work with constant hydraulic parameters in their modeling.

Thus, it is extremely important to have more improved physical models, in which they add more information in the formulation and that are of physical importance. However, for a more robust model, more complex solution techniques are required to resolve.

Thus, the objective of this work is to present an analytical solution for the models of dispersion of pollutants in water bodies, which brings more information to the field of turbulence, since many studies show that turbulence is not homogeneous in these types of problems. The purpose of this work is to apply the Generalized Integral Laplace Transform Technique technique, GILTT (Moreira *et al.*, 2009; Buske *et al.*, 2011), to obtain the solution for dispersion models in water bodies. Some works have already been applying this technique to simulate controlled tank experiments (Oliveira, 2015; Machado, 2019), however in this work the technique will be applied to simulate an experiment carried out on the Paraibuna river, state of Minas Gerais, that is, a real and more complex environment. This experiment aimed to evaluate the transport and dispersion capacity of the Paraibuna River, using fluorescent tracers (Soares *et al.*, 2006).

2. THE MODEL

The equation that describes the problem of dispersion of a contaminant in a water body is obtained from the law of conservation of mass. In this work, the Eulerian model will be used to describe the concentration field, simulating the entire concentration profile through a fixed reference system. The polluting source was considered as a reference point. For the development of this work, a uniform flow was considered, according to Soares *et al.* (2006). Thus, the basic equation that defines the dispersion and one-dimensional (longitudinal) transport of a conservative pollutant is represented by the equation:

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = D_x\frac{\partial^2 C}{\partial x^2}. \tag{1}$$

Here $C(x,t)$ in (mg/m^3) represents the average concentration of the pollutant, U the component of the average speed in the longitudinal direction in (m/s) and D_x in (m^2/s) the turbulent diffusion coefficient longitudinal.

The initial and boundary conditions used are shown below:

$$C(x,t=0) = \frac{M}{A}\delta(x); \tag{2}$$

$$\left.\frac{\partial C}{\partial x}\right|_{x=0} = 0; \tag{3}$$

$$C(L_x,t) = 0. \tag{4}$$

In the Eq. 1 - 11, A is the wet area (m^2) and M is the amount of pollutant released. Note that the source condition is represented by a dirac delta (δ), this condition means that an instant $t = 0$ an amount M of the pollutant was released in (mg). For the domain under study, it was considered $0 \leq x \leq L_x$.

Solving by GILTT, initially the Sturm-Liouville problem is associated with the original problem:

$$\Psi''(x) + \lambda^2\Psi(x) = 0, \qquad \Psi'(0) = 0, \qquad \Psi(L_x) = 0. \tag{5}$$

Therefore, the general solution for the Ordinary Differential Equation (ODE), Eq. (5), is:

$$\Psi(x) = c_1\cos(\lambda x) + c_2\sin(\lambda x). \tag{6}$$

Applying the boundary conditions (in $x = 0$ and $x = L_x$), therefore, the solution to the auxiliary problem is given by:

$$\Psi_n(x) = \cos(\lambda_n x), \tag{7}$$

with $\lambda_n = \frac{(n-1/2)\pi}{L_x}$ to $n = 1, 2, 3, \ldots$. Then, the concentration of pollutants is expanded in a series , based on the Sturm-Liouville problem:

$$C(x,t) = \sum_{n=1}^{\infty}\Psi_n(x)c_n(t). \tag{8}$$

Substituting the expansion in the Eq. (8) in the Partial Differential Equation (PDE), obtain:

$$\sum_{n=1}^{\infty}\Psi_n(x)c'_n(t) + U\sum_{n=1}^{\infty}\Psi'_n(x)c_n(t) = D_x\sum_{n=1}^{\infty}\Psi''_n(x)c_n(t). \tag{9}$$

The associated Sturm-Liouville problem, it has $\Psi''_n(x) = -\lambda_n^2\Psi_n(x)$ and therefore:

$$\sum_{n=1}^{\infty}\Psi_n(x)c'_n(t) + \sum_{n=1}^{\infty}\big(U\Psi'_n(x) + D_x\lambda_n^2\Psi_n(x)\big)c_n(t) = 0. \tag{10}$$

Applying the integral operator $\int_0^{L_x}(\,.\,)\Psi_m(x)\mathrm{d}x$ in the Eq. (10):

$$\sum_{n=1}^{\infty}\int_0^{L_x}\Psi_n(x)\Psi_m(x)\mathrm{d}x c'_n(t) + \sum_{n=1}^{\infty}\int_0^{L_x}\big(U\Psi'_n(x) + D_x\lambda_n^2\Psi_n(x)\big)\Psi_m(x)\mathrm{d}x c_n(t) = 0. \tag{11}$$

Rewriting in matrix form, assuming that $Y(t)$ is a vector of components of $c_n(t)$ and considering that:

$$e_{n,m} = \int_0^{L_x}\cos(\lambda_n x)\cos(\lambda_m x)\mathrm{d}x, \tag{12}$$

$$b_{n,m} = \int_0^{L_x} \big[-U\lambda_n \sin(\lambda_n x)\cos(\lambda_m x) + D_x \lambda_n^2 \cos(\lambda_n x)\cos(\lambda_m x)\big] \mathrm{d}x. \tag{13}$$

Equation (11) written in matrix form is given by:

$$E.Y'(t) + B.Y(t) = 0. \tag{14}$$

Because E is a diagonal matrix can determine its inverse, so Eq. (14) can be rewritten as:

$$Y'(t) + F.Y(t) = 0, \tag{15}$$

in which $F = E^{-1}.B$.

As an initial condition for the matrix equation, the source condition is used:

$$C(x, t = 0) = \frac{M}{A}\delta(x). \tag{16}$$

Expanding $C(x, 0)$ in terms of the eigenfunctions of the Sturm-Liouville problem and using the orthogonality property of these functions, it has:

$$c_n(0) = E^{-1} \int_0^{L_x} \frac{M}{A}\delta(x)\cos(\lambda_n x)\mathrm{d}x, \tag{17}$$

thus, the initial condition $Y(0) = [c_n(0)]$, where the components are $c_n(0)$, can be calculated by the Eq. (17).

Then, the matrix equation will be solved by diagonalization and by Laplace transform. Therefore, to solve the matrix ODE, initially the diagonalization is applied in F, writing:

$$F = XD_iX^{-1}, \tag{18}$$

where X is the matrix of the eigenvectors, D_i is the diagonal matrix of the eigenvalues of the matrix F and X^{-1} is the inverse of the matrix X. Thus, the Eq. (15) becomes:

$$Y'(t) + XD_iX^{-1}.Y(t) = 0. \tag{19}$$

Applying the Laplace transform to the time variable, $L\{Y(t), t \to s\} = \overline{Y}(s)$, obtém-se:

$$sI\overline{Y}(s) - Y(0) + XD_iX^{-1}.\overline{Y}(s) = 0. \tag{20}$$

Isolating the $\overline{Y}(s)$ in the algebraic equation:

$$\overline{Y}(s) = X(sI + D_i)^{-1}X^{-1}Y(0). \tag{21}$$

To determine $Y(t)$, apply the Laplace inverse transform and arrive at:

$$Y(t) = X\,\underbrace{L\{(sI + D_i)^{-1}\}}_{G(t)}\,X^{-1}Y(0), \tag{22}$$

in which:

$$G(t) = \begin{bmatrix} e^{-d_1 t} & 0 & \dots & 0 \\ 0 & e^{-d_2 t} & \vdots & \vdots \\ \vdots & 0 & \ddots & 0 \\ 0 & 0 & \dots & e^{-d_n t} \end{bmatrix}. \tag{23}$$

Finally, one obtains the solution for the vector $Y(t)$ given by the equation:

$$Y(t) = XG(t)X^{-1}Y(0). \tag{24}$$

Note that when determining the vector $Y(t)$, we know the components $c_n(t)$, so the solution for the concentration given by the Eq. (8) is well determined, that is, the solution of the concentration is

$$C(x, t) = \lim_{N \to +\infty} \sum_{n=0}^{N} \Psi_n(x)c_n(t), \tag{25}$$

in which $\Psi_n(x) = \cos(\lambda_n x)$ and $\lambda_n = \frac{(n-0.5)\pi}{L_x}$ are obtained through the Sturm-Liouville problem associated with the original problem and $c_n(t)$ is obtained through the partial differential equation (PDE) using Laplace transform and the initial condition of the problem. More details of the GILTT method can be found in (Moreira *et al.*, 2009).

3. RESULTS AND DISCUSSIONS

The Gaussian solution for this type of problem is also presented to compare the results:

$$C(x,t) = \frac{M}{2A\sqrt{\pi D_x t}} e^{-\frac{(x-Ut)^2}{4D_x t}} \tag{26}$$

It is worth mentioning that in the solution obtained by the GILTT technique, it can be considered that the turbulence (D_x) and the flow profile (U) vary along the path.

To make an analysis of the transport and diffusion models in water bodies, it is recommended to conduct a study on their capabilities to correctly describe real situations (Moreira *et al.*, 2005).

As mathematical modeling is an important tool for assessing environmental impact, this research aims to present an analytical model for dispersion of pollutants by GILTT methodology. In this section, simulations will be presented for the evaluation and discussion of the model obtained, the data for the analysis of the characteristics of dilution and transport of pollutants was provided by the EDT 159/05 report by the authors Soares, Ribeiro and Guedes (2011), in which it was carried out field simulations with using fluorescent tracers on the Paraibuna river.

The experiment used was conducted in an attempt to answer the consequences arising from the dispersion of products in the liquid medium, as well as the need for predicting the pollutant cloud's arrival with as soon as possible in important sites located close to the pollution source.

Thus, the experiment aimed main to quantify the characteristics of dilution and transport of pollutants in the Paraibuna River using fluorescent tracers Amidorodamine G Extra e Fluoresceína Sódica (also known as Uranina) for two different flows.

According to the 159/05 report by the authors Soares, Ribeiro and Guedes (2011), the *in situ* experiment was carried out using tracers called fluorescent dyes used in hydrology research. For this work, experiments with the tracer Amidorodamine G Extra were used: a substance that is not very sensitive to degradation by light, the action of bacteria and adsorption, a characteristic that facilitates hydrological studies in surface waters.

It is noted that the application of tracers is still being used to understand the behavior of surface and groundwater, both in the country and abroad.

In a recent article Ferreira et al (2018) studied the interaction of the cenozoic sediments in the São Paulo Aquifer with the uranine fluorescent tracer.

According to this article, fluorescent dyes are defined as organic compounds that show fluorescence, in the case of this work, the tracer used was that of uranine, also known as sodium fluorescein or acid yellow 73.

According to the article, among the various fluorescent dyes available on the market, dyes are preferable in hydrological and hydrogeological studies because they are, for example: soluble in water, easily detectable due to their strong fluorescence, non-toxic in low concentrations and other characteristics that contribute to studies in the aquatic environment.

Also noteworthy is a study with fluorecent tracer in an aquifer in China, the article by Yang et al (2019) aiming to assess the impacts on the Jinfoshan karst aquifer, of the septic effluents of the Hotel *Jinfoshan Holiday of Chongqing* , where tests were performed with fluorescent tracer.

Good acceptance and results are observed in the assessment of environmental impacts and in hydrological studies using fluorescent tracers, such as uranine, mentioned in the case study that serves as the basis for this research.

It is noteworthy that this is a conservative contaminant. This means that it does not react with other pollutants, its concentration is not altered by physical, chemical and biological processes, and its concentration in aquatic environments decreases only through the processes of advection and diffusion.

Following, according to the 159/05 report, the monitoring and injection sections of the Amidorodamine G Extra tracer are presented:

- Section 0 (Injeção): Bridge over the Paraibuna river, located at km 777 of BR-040 - Industrial District of Juiz de Fora;
- Section 1 (Represa): Bridge over the Paraibuna river, located at Rua Honório de Brito - Bairro Barbosa Lage;
- Section 3 (Pontilhão): Bridge over the Paraibuna River, between Benjamin Constant and Halfeld streets;
- Section 4 (Posto Policial): Bridge over the Paraibuna river, located in the Bairro Vila Ideal in front of the Curtume Surerus;

Table 1 presents a summary of the locations of the tracer monitoring sections in relation to the distance from the injection point.

Table 1. Injection and monitoring section data synthesis

Sections	Distance in km from the injection point	denomination
S0	0.0	Injeção
S1	7.6	Represa
S2	16.0	Pontilhão
S3	20.0	Posto Policial

Source: based on data from the report by Soares, Ribeiro and Guedes. (2011).

In the Fig. 1, it is possible to view the monitoring sections of the tracers in the Paraibuna River:

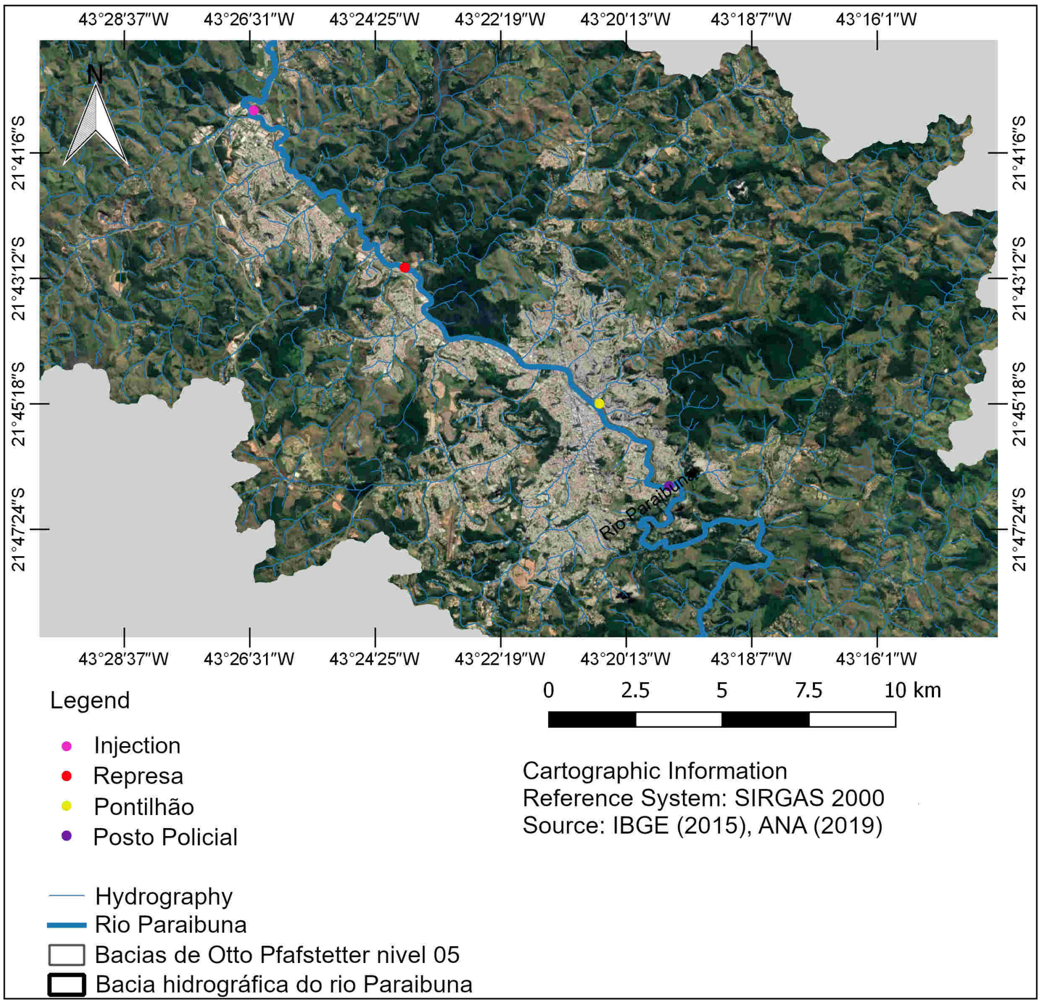

Figure 1. Mapped location of monitoring sections on the Paraibuna River

Source: produced by the authors of this article.

Figure 1 shows the monitoring sections of the tracers on the Paraibuna River, a figure created based on the hydrographic data available on the IBGE and ANA websites.

The development of the field campaign took place on October 7, 2005, and briefly a mass of $500g$ of tracer was injected at a flow rate of $23.20(m^3/s)$.

It should be noted that the flow corresponds to the average value measured at the Juiz de Fora Jusante fluviometric station.

The injection of the tracers was carried out in the section of the river located at km 777 of BR 040, Bairro Benfica, being at 05:45 h. Regarding the temperature values, no major variations were detected in the monitored river, the average temperature was in the range of 23.5^0C.

Table 2 shows the measures of the experiment used to evaluate the partial results of the study:

Table 2. Experimental campaign measures 1

Local	Wet area (m^2)	Flow rate (m^3/s)	Injection point distance (m)	Average speed (m/s)	Turbulent diffusion coefficient (m^2/s)
S1	30.138	15.67	7600	0.52	6.2
S3	37.092	19.55	16000	0.527	11.0
S4	33.678	18.62	20000	0.553	12.7

Source: authors based on data from the Soares, Ribeiro and Guedes report (2011).

In this study, results are presented for dispersion of Amidorodamine G Extra. The stretch of the river studied is located between the Industrial District, located in Benfica district , and extends for 27 kilometers to the hydroelectric power plant Marmelos Zero, located in the Retiro district, Juiz de Fora city.The period of realization of the campaigns took place between October 7 and December 1, 2005.

The Fig.2 presents graphs with the concentration convergence for the GILTT model. According to the number of terms (N) of the series expansion of the solution (Eq. (25)), were considered $N = 20$, $N = 40$, $N = 80$ and $N = 160$. The graphs show the evolution of the concentration at the position $7600m$ away from the pollutant release site. In the graphs is also presented the Gaussian solution and the observed data of the experiment.

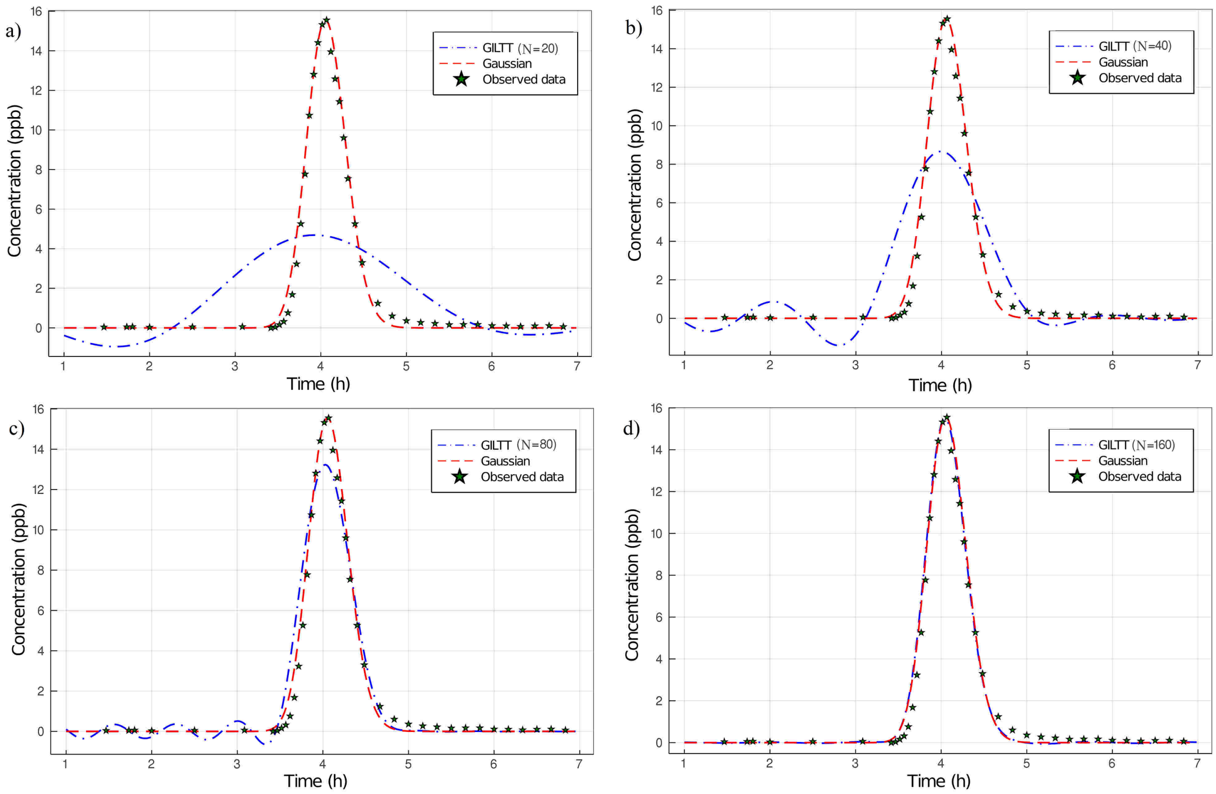

Figure 2. Convergence of concentration to the GILTT model, considering a) $N = 20$, b) $N = 40$, c) $N = 80$ e d) $N = 160$ in Eq. (14)

From $N = 160$ the GILTT solution converges to the analytical solution (Gaussian). Thus, it was used for all simulations $N = 160$. As both methods are analytical, the two solutions must converge on the same curve, as shown in Fig. 2d. It is also observed in Fig. 2d the good proximity of the analytical solutions to the observed data, the points being practically located on the curves.

The following is presented the comparison, in Fig. 3, of the Gaussian and GILLT models with the data observed in three different positions ($x = 7600m$, $x = 16000m$ and $x = 20000m$).

In Fig. 3 are considered as distribution curves at the three experiment collection points: at the dam (at $x = 7600m$); at the bridge (at $x = 16000m$) and at the police station (at $x = 20000m$). For a verification of the models were plotted

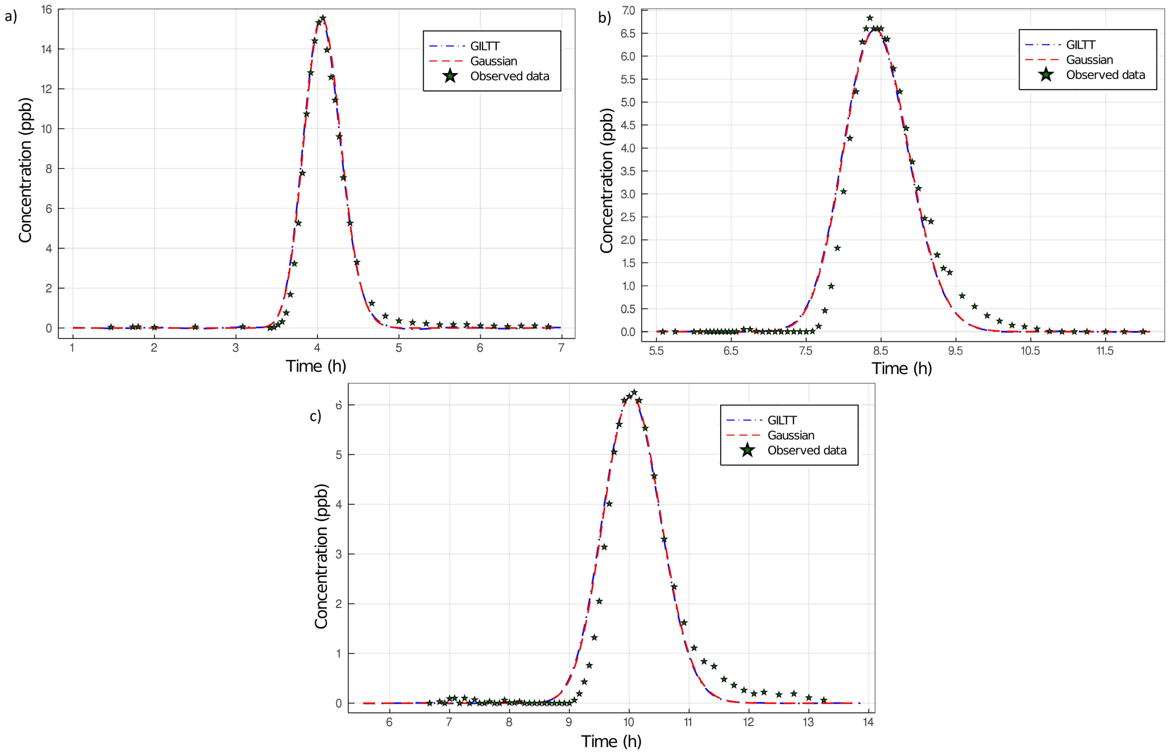

Figure 3. Concentration distribution curves (from the tracer Amidorodamine G Extra) of the GILTT and Gaussian models, compared with the data observed at the dam position: a) $x = 7600m$ b) $x = 16000m$ and c) $x = 20000m$

the observed data. For an ideal model the curves of the analytical models should be on the observed data (stars). In the figures presented, it can be seen that the models are satisfactorily representing the observed data.

The figures also show the moments at which the concentration peaks occur in the locations under analysis, for example, in Fig. 3c it is possible to verify, through the models, that the maximum concentration occurs in $t \approx 10h$ and that the concentration is close to $6.2ppb$. Figure 3 show that the distribution curve has a flattening as it moves away from the source (point of origin of the pollutant release), this happens due to the influence of turbulent diffusion.

4. CONCLUSIONS

The initial results show that the GILTT solution has the same behavior as the Gaussian solution, as expected, since they are two analytical solutions to the problem. The comparisons of the curves with the experimental data show a good agreement between the models and the experiment. It is intended to make a statistical analysis of the model, to confirm this good agreement. The great advantage of the GILTT method when compared to the Gaussian method is that the turbulent diffusion coefficient and the flow profile of the river can vary along the route, which makes it more realistic model.

In the next steps, it is intended to deepen the verification of works related to the theme of modeling in rivers and channels, with the purpose of this study serving as a basis for future works in the area of modeling and as support for companies working in the area of evaluation environmental impacts.

Finally, it should be noted that these partial results, which confirm the good agreement between the analytical solutions and the experiment data, do not exhaust the need for research, since the study of a mathematical model, the execution and confirmation of the experiments with realistic data , are extremely necessary in view of the objective of analyzing ways to control pollutants ensuring their applicability before real use, as we are dealing with the environment and with the necessary resources for our survival.

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