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Efficient Statistical Tools for the Estimation of the Longitudinal Dispersion Coefficient

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***Keywords* — Bayesian approach, Longitudinal dispersion coefficient, Markov Chain Monte Carlo method, Tracer flow, Transporting pollutants.**

***Abstract* — The problem of transporting pollutants in natural rivers can be modeled using saline tracer injection techniques, which are very useful for obtaining important information related to water quality in river stretches, such as the physical parameter longitudinal dispersion coefficient. The objectives of this work are to formulate an inverse problem for the tracer flow process in natural rivers using a Bayesian approach to update the longitudinal dispersion coefficient, and use the Markov Chain Monte Carlo (MCMC) to solve the inverse problem formulated.*

I. INTRODUCTION

The possibility of applying techniques favorable to a behavioral prognosis in several areas of knowledge motivates the use of statistics as a tool to support decision-making, which is justified by its ability to help in the analysis and interpretation of data. Thus, statistics are present in several studies and applications in the areas of engineering, exact sciences, biological sciences, and health sciences [1, 8, 10, 13, 14, 15, 16, 17, 20, 21, 22, 26, 27, 31], given that the Probabilistic analysis can be understood as the study of predicting the behavior of a single variable, or a set of variables in a specific scenario. Therefore, its conception consists of quantifying the uncertainty associated with the occurrence phenomenon.

Currently, the preservation of natural systems is considered one of the challenges of Brazilian society, with water being one of the environmental factors that have caused considerable concern among professionals working in this area [29]. It is known that the quality of water depends on the actions of man and various natural conditions, and knowledge of its information becomes essential for the management of water resources. Lack of knowledge of water quality increases uncertainties in future decision-making, which in turn has negative consequences in the management of water resources [29].

The use of tracer injection techniques in a given location of the watercourse has been widely used in studies of problems related to the transport of pollutants in natural rivers, to seek important information on water quality, such as, for example, the physical parameter longitudinal dispersion coefficient. The mathematical model that describes this physical flow process is composed of a partial differential equation subject to the certain boundary and initial conditions.

Several methods in the literature can be used to determine the longitudinal dispersion coefficient [25, 26] present in the mathematical model that describes the physical process of tracer flow in natural rivers. However, this work proposes a Bayesian methodology together with the Markov Chains Monte Carlo method as an alternative to traditional methods for estimating the parameter of unknown interest.

The Bayesian methodology is based on one of the most important mathematical formulations of probability theory, known as Bayes' theorem, which updates the information of the parameter of unknown interest, taking into account the a priori information about the parameter of interest and the known information about the observed sample [2, 5, 9, 15, 23].

To solve the inverse Bayesian problem of transporting pollutants in natural rivers, the Markov Chain Monte Carlo (MCMC) stochastic method can be used, which is based on specific algorithms to simulate ergodic Markov Chains whose stationary distribution (or equilibrium distribution) is the posterior probability distribution of interest [5, 9, 15, 23]. Among the various specific algorithms used by the MCMC method to generate the Marvok Chains, the special case of the Metropolis-Hastings algorithm [13, 21] based on random walk [4, 5, 9, 15, 23] is used in this work, which proposes the new point candidate (longitudinal dispersion coefficient) considering the current previously simulated longitudinal dispersion coefficient value plus a random increment.

The motivation of this proposal is that the Bayesian methodology together with the Markov Chain Monte Carlo method is an attractive and efficient statistical tool, which has significantly contributed to the scientific and technological development of several areas of knowledge, for example, in the estimation of the physical parameter (permeability) in fluid flow problems in porous media [3, 4, 5, 6, 7, 11, 12, 15, 20].

In this sense, it is expected that the study presented in this research paper can significantly contribute to problems related to the monitoring and preservation of natural rivers that receive some type of liquid waste with harmful properties to the environment, which can cause changes in the ecosystem and negatively impact the entire its dependent chain. More details on the environmental problems described above can be found in the literature [24, 29, 30].

II. MATHEMATICAL MODELING

Considering a rectangular domain $\Omega \in R$ limited in region $[0, L_x]$ x $[0, L_y]$ in the contour $\partial\Omega$, with $L_x[m]$ and $L_y[m]$ the physical dimensions of the river in the and directions x e y, respectively. Here $c = c(\boldsymbol{x}, t)[mg/l]$ is the concentration of the tracer at the point $\boldsymbol{x} = (x, y)$ in the instant of time $t[s]$.

The mathematical model that describes the physical process of transporting contaminants in river with domain Ω, over a span of time $I = [0, T]$, with $t \in I$, is described by the following partial differential equation [28]:

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = E_l\frac{\partial}{\partial x}\left(\frac{\partial c}{\partial x}\right) + E_t\frac{\partial}{\partial y}\left(\frac{\partial c}{\partial y}\right), \tag{1}$$

where in this equation u is velocity river water, expressed in m/s; $E_l$is longitudinal dispersion coefficient, expressed in m^2/s; e E_t é o longitudinal dispersion cross, expressed in m^2/s. The Eq. (1) is subject to the following boundary conditions [28]:

$$\begin{aligned} &c(x, y, t) = c_0; x = 0, 0 \le y \le L_y, t > 0,\\ &\frac{\partial c(x, y, t)}{\partial x} = 0; x = L_x, 0 \le y \le L_y, t > 0,\\ &\frac{\partial c(x, y, t)}{\partial y} = 0; y = 0, 0 \le x \le L_x, t > 0,\\ &\frac{\partial c(x, y, t)}{\partial y} = 0; y = L_y, 0 \le x \le L_x, t > 0, \end{aligned} \tag{2}$$

and initial

$$c(x, y, 0) = c_1(x, y); 0 \le x \le L_x, 0 \le y \le L_y. \tag{3}$$

In Fig. 1 we find the schematically represents the flow problem in geometry Ω, subject to boundary conditions (2).

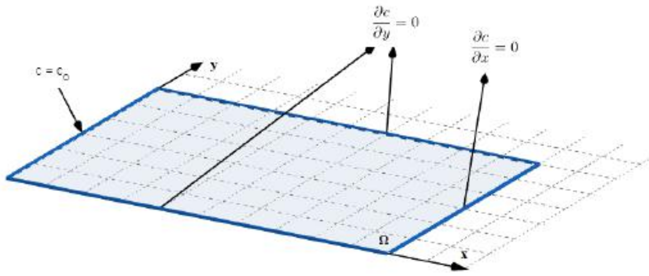

Fig. 1: Discretization and boundary conditions in the domain.

To solve the partial differential equation (1) subject to conditions (2) - (3), which governs the transport of pollutants in river stretches, the Finite Volume method is used, with implicit formulation, which performs the spatial and temporal integration in each volume of control v_c. It, is the variables to be calculated are located at the center and borders of each v_c, resulting in a linear system [18,19]. In the advective term, an interpolation of the type is used Upwind (UDS), to calculate the values of the variables of each border in relation to the variable located in the center of the volume of control [18, 19]. To solve the linear system resulting from the discretization of the Finite Volumes method, whose coefficient matrix presents a characteristic of a sparse matrix, the Thomas Algorithm (Tridiagonal Matrix Algorithm) is used, which originates from the Gaussian elimination method [18, 19].

III. METHODOLOGY

This section presents the formulation of the inverse problem for the flow process of tracers in river stretches using a

Bayesian approach to update the parameter of interest (longitudinal dispersion coefficient - E_l). The MCMC method used to solve the inverse problem proposed in this research work is presented, which in turn estimates the parameter E_l. It is worth noting that the methodology used in this research paper was based on the work of [15].

3.1 Bayesian approach

This section presents the Bayesian methodology that will be used to update the longitudinal dispersion coefficients E_l, taking into account the a priori information on the parameter of interest E_l and the known information about the observed sample.

Based on the work of [15], it is proposed to define the set of observed values of the tracer concentration in fluvial stretches (or reference values) as:

$$O(c_o) = \{c_o(\boldsymbol{x}_1, t_j); j = 1,\cdots, N_t\}, \tag{4}$$

where $\boldsymbol{x}_1$denotes the location of the collection point in the region Ω; and N_t denotes the number of times the tracer concentration c_o is evaluated over timet_j, with $j = 1,\cdots, N_t$ (see Fig. 2).

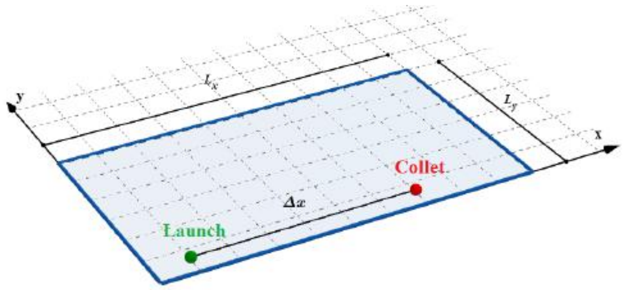

Fig. 2: Simplified model of the study region with launch and collection points.

An update of the information of the parameter of interest E_l is performed through the Bayes' theorem expressed by [15]:

$$P(E_l|O(c_o)) \propto P(O(c_o)|E_l)P(E_l), \tag{5}$$

where $P(E_l|O(c_o))$ is posterior distribution of the parameter of interest E_l; and the o factor $P(O(c_o)|E_l)$ is the likelihood function, which represents the contribution of $O(c_o)$ on the parameter E_l and, in the case of this work, it is considered as a normal distribution expressed by [15]

$$P(O(c_o)|E_l) \propto exp\left\{\frac{-\mathcal{E}}{2\sigma^2}\right\}, \tag{6}$$

where $\mathcal{E}$ *is* the error defined by [15]:

$$\mathcal{E} = \sum_{j=1}^{N_t}\left[c_s(\boldsymbol{x}_1, t_j) - c_o(\boldsymbol{x}_1, t_j)\right]^2, \tag{7}$$

where, $c_s(\boldsymbol{x}_1, t_j)$ is the simulated concentration of the tracer at the collection point $\boldsymbol{x}_1$ for the instant of time t_j; and σ^2 is the accuracy associated with concentration measurements $c_s(\boldsymbol{x}_1, t_j)$ and $c_o(\boldsymbol{x}_1, t_j)$.

As E_l will be proposed from a normal distribution with mean $\mu_p = 0$ and variance $\sigma_p^2 = 1$, then it is assumed that the prior distribution of the parameter of interest E_l is [15]:

$$P(E_l) = exp\left\{\frac{-[E_l - \mu_p]^2}{2\sigma_p^2}\right\}. \tag{8}$$

3.2 Markov Chain Monte Carlo method

In the formulation of the inverse problem presented in Subsection 3.1, the Markov Chain Monte Carlo (MCMC) method is based on stochastic simulations, which has been shown to be an efficient technique for solving several complex problems [3, 4, 5, 6, 7, 10, 11, 12, 15, 20]. The MCMC method uses specific algorithms to generate ergodic Markov Chains whose stationary distribution is the posterior distribution $P(E_l|O(c_o))$.

In this work we consider the Metropolis-Hastings algorithm based on random walk to build the Markov Chains [15]:

$$\left\{E_l^{(k)}: k \in K\right\}, \tag{9}$$

which proposes a new candidate E_l given by:

$$E_l = E_l^{(k)} + (h_{rw}) * z, \tag{10}$$

where K is the set of non-negative integers; $E_l^{(k)}$ is the current state of the Markov Chain (or state of the Markov Chain in the instant k); h_{rw} is the parameter that determines the step size of the Markov Chain; and z has a Gaussian distribution $N(\mu_p, \sigma_p^2)$, with $\mu_p = 0$ and $\sigma_p^2 = 1$. The probability of acceptance of the new candidate E_l is given by [15]:

$$\alpha(E_l|E_l^{(k)}) = \begin{cases} min\left(\dfrac{P(E_l|O(c_o))q(E_l^{(k)}|E_l)}{P\left(E_l^{(k)}\middle|O(c_o)\right)q(E_l|E_l^{(k)})}, 1\right), A \\ 1, B \end{cases} \tag{11}$$

where

$$A = P\left(E_l^{(k)}\middle|O(c_o)\right)q(E_l|E_l^{(k)}) > 0$$

and

$$B = otherwise,$$

such that $E_l^{(k+1)} = E_l$ with probability $\alpha\left(E_l \middle| E_l^{(k)}\right)$ and $E_l^{(k+1)} = E_l^{(k)}$ with probability $1 - \alpha\left(E_l \middle| E_l^{(k)}\right)$. It is worth noting that the factor $q(*)$ is the instrumental probability distribution. For a better understanding of the MCMC method, Algorithm 1 is presented.

Algorithm 1: The MCMC method.

Step 1: Set $\boldsymbol{k = 0}$ and specify an initial value for the longitudinal dispersion coefficient $\boldsymbol{E_l^{(0)}}$, such that

$\boldsymbol{P\left(E_l^{(0)} \middle| O(c_0)\right) > 0}$.

Step 2: Generate a new candidate $\boldsymbol{E_l \sim q\left(E_l \middle| E_l^{(k)}\right)}$, according (10).

Step 3: Solve the tracer flow problem modeled by Eq. (1) subject to conditions (2) - (3).

Step 4: Calculate the probability of acceptance of the new candidate $\boldsymbol{E_l}$, according (11).

Step 5: Generate $\boldsymbol{w}$ from the uniform distribution in the interval $[\boldsymbol{0}, \boldsymbol{1}]$, this is $\boldsymbol{w \sim U(0, 1)}$.

Step 6: If $\boldsymbol{w \leq \alpha\left(E_l \middle| E_l^{(k)}\right)}$, then

$\boldsymbol{E_l^{(k+1)} = E_l}$,

otherwise

$\boldsymbol{E_l^{(k+1)} = E_l^{(k)}}$.

Step 7: Increment $\boldsymbol{k = k + 1}$, return to **Step 2** and continue the procedure until convergence is achieved.

IV. NUMERICAL RESULTS

4.1 Simulation parameters for observed values

For the construction of the set of observed values of the tracer concentration in fluvial stretches (or reference values), according to Eq. (4), the parameters considered the most adequate to the real problem are used [28]. Thus, a saline tracer (NaCl) was used, where the mean concentration of salinity (NaCl) in the natural river is determined at 37 mg/l. The launch point of the plotter is 0.7 m from the bank. At this point, the saline concentration became 2,551 mg/l at the time of release. The collection point was kept at the same distance from the river bank, however, carried out 50 meters downstream.

The domain Ω that represents the surface of the river, has dimensions L_x and L_y corresponding to 182 m and 42 m, respectively. This region is discretized with a mesh of 260 x 60 elements, resulting in a total of 15,600 volumes with a 0.7 m edge each. The simulation was parameterized with a maximum time of 352 seconds, and the time step used to solve Eq. (1) was equal to 2 seconds.

Finally, it is considered the speed of the river water u equal to 0.359 m/s; the transversal dispersion coefficient E_t equal to 0.008 m^2/s; and the longitudinal dispersion coefficient E_l equal to 0.33 m^2/s (reference value of the coefficient).

4.2 Results and discussions

This subsection is reserved to present the numerical results obtained with the Markov Chain Monte Carlo method for solving the Bayesian inverse problem. The values of the simulated concentration of the tracer $c_s(\boldsymbol{x}_1, t_j)$ were obtained using the same parameters presented in Subsection 4.1, with the exception of the value adopted for the longitudinal dispersion coefficient.

Was specify $10.0\ m^2/s$ for initial value for the longitudinal dispersion coefficient $E_l^{(0)}$. For the parameter that determines the step size of the Markov Chain in Eq. (10) was used $h_{rw} = 0.01$. The value of the σ^2 in Eq. (6) was fixed at 0.25 for all simulations, and the tracer concentration $c_s(\boldsymbol{x}_1, t_j)$ was evaluated at each two seconds of simulation.

The numerical results were obtained from a maximum of 10,000 proposals, with the objective of selecting 1,500 accepted samples of the longitudinal dispersion coefficient. The tracer concentration $c_s(\boldsymbol{x}_1, t_j)$ was evaluated at each 2 seconds of simulation, with a maximum time of 352 seconds. It is observed that to reach the quantity of 1,500 accepted samples, 8,897 proposed samples needed only, thus resulting in an acceptance rate of 16.85%.

In Fig. 3 are presented the variations of the tracer concentration errors values for the 1,500 samples accepted, according to Eq. (7). Making a visual analysis of Fig. 3, it can be seen that the Markov Chain generated by the MCMC method converges to the stationary distribution of interest, which in this case it is the posterior distribution [15]. It is noticed that shortly after the 1,000 accepted samples, more precisely in the 1,184 sample, the curve reaches an stability zone. Thus, there is a set of 316 accepted samples of the longitudinal dispersion coefficient, after burn-in (1,184 accepted samples).

It can be observed a significant reduction in tracer concentration errors, reaching values below 5 measurement units. This can be seen in more detail in Fig. 4, which is presented the zoom of stability region of Fig. 3, this is, quantitative samples accepted from 1184 to 1500.

The reduced values of the simulated tracer concentration errors indicate that the values of the accepted longitudinal dispersion coefficients are close to the value of the reference coefficient used to generate the observed tracer concentration at the collection point $\boldsymbol{x}_1$ at each instant of time t_j.

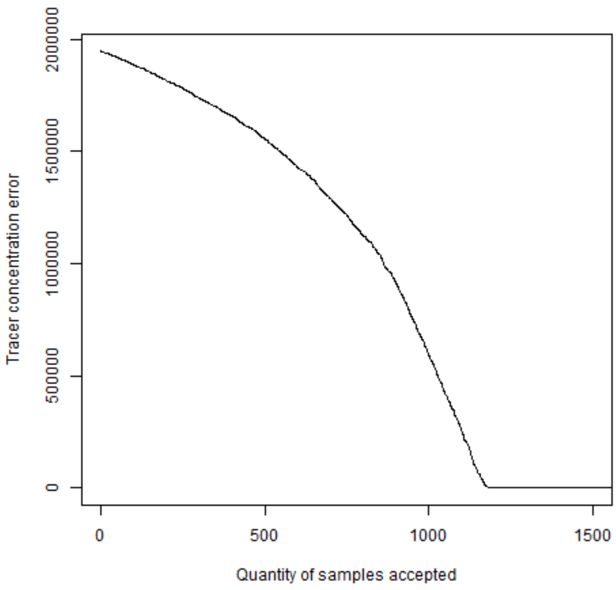

Fig. 3: Tracer concentration error versus quantity of samples accepted.

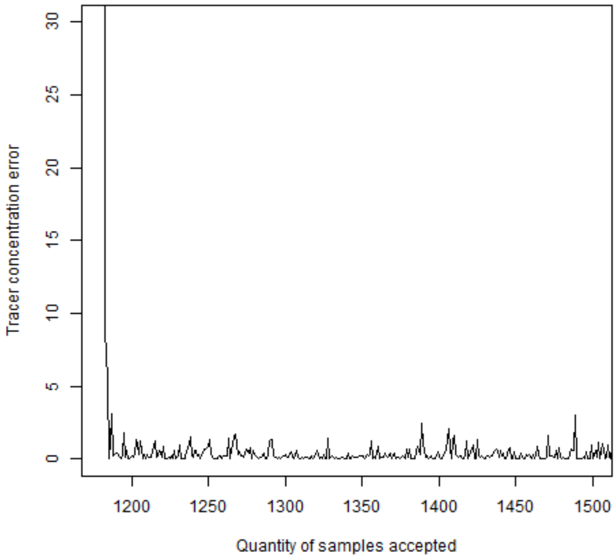

Fig. 4: Zoom of Fig. 3. Quantitative samples accepted from 1184 to 1500.

In Fig. 5 are presented the samples accepted of longitudinal dispersion coefficients E_l, through the MCMC method and Metropolis-Hastings algorithm based on random walk. In Fig. 6 are presented the zoom of stability region of Fig. 5, this is, quantitative samples accepted from 1184 to 1500.

Compared to the initial value for the longitudinal dispersion coefficient $E_l^{(0)}$, it is observed in Fig. 5 that the values of the accepted coefficients decrease considerably as the number of accepted samples increases, reaching values close to the reference coefficient after a burn-in of 1184 accepted samples (see Fig. 6). In fact, as were mentioned earlier, this factor contributes to obtaining a reduced values of the simulated tracer concentration errors. Furthermore, it is noted in Fig. 6 that the MCMC method selects distinct longitudinal dispersion coefficients.

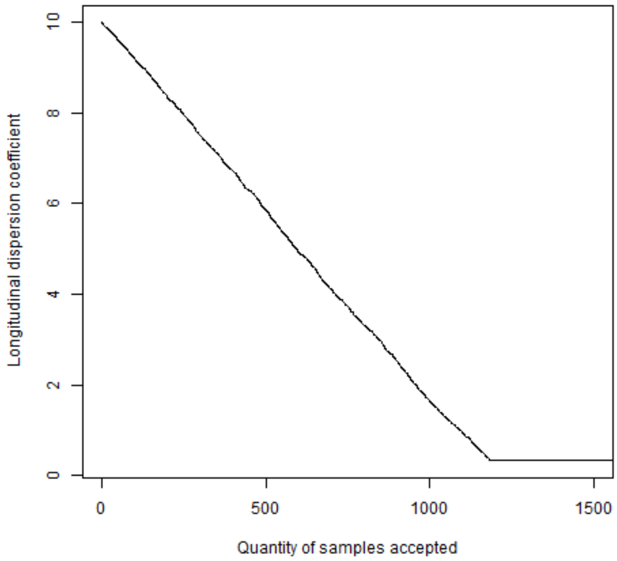

Fig. 5: Longitudinal dispersion coefficient versus quantity of samples accepted.

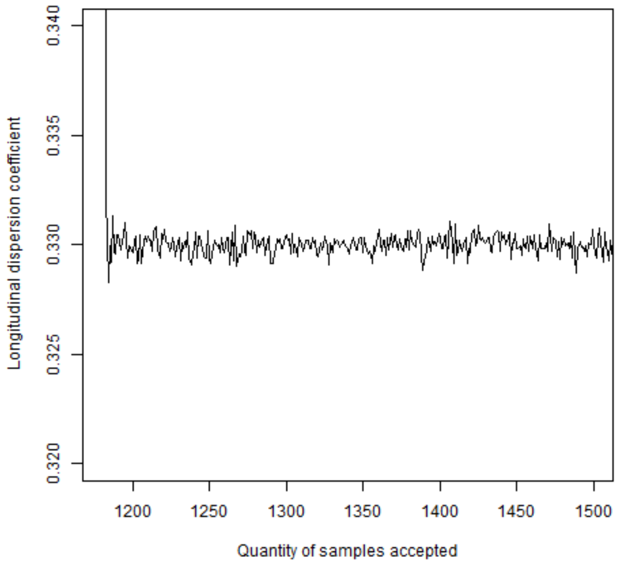

Fig. 6: Zoom of Fig. 5. Quantitative samples accepted from 1180 to 1500.

In Figs. (7) – (10) are presented the tracer concentration profiles at the $\boldsymbol{x}_1$ position, which represents the location of the collection point in region Ω. In these figures, the solid red lines correspond to the tracer concentration values obtained with the reference longitudinal dispersion coefficient

$E_l = 0.33\, m^2/s$; the solid green lines correspond to the values of the tracer concentrations obtained with the initial longitudinal dispersion coefficient $E_l^{(0)} = 10\, m^2/s$; and the solid blue lines correspond to the mean values of tracer concentrations obtained for a limited set of accepted samples.

For a better analysis of the behavior of the tracer concentration profiles, the graphs with the respective mean profiles were divided into groups with the quantitative of 50 (see Fig. 8), 150 (see Fig. 9) and 250 (see Fig. 10) accepted samples of the longitudinal dispersion coefficient after the heating period, and also a group of with the quantitative of 50 samples accepted before the burn-in period (see Fig. 7). Thus, it becomes possible to better understand the mean results of tracer concentrations close to the reference values observed at the collection point $\boldsymbol{x}_1$.

Note that there is a significant difference between the tracer concentration profiles determined by the reference (solid red lines) and initial (solid green lines) coefficients. In fact, this is due to the large difference between the values of the reference and initial longitudinal dispersion coefficients.

It can be seen in Fig. 7 that the mean tracer concentration profile (solid lines in blue) behaves very similarly and close to the reference concentration values, even considering the mean of the last 50 samples before the burn-in period.

However, it is observed in Figs. 8 - 10 that the MCMC method was able to obtain better results than those presented in Fig. 7. In fact, this is because the average tracer concentration profiles (solid blue lines) corresponding to simulations performed using 50, 150 and 250 samples accepted of the dispersion coefficient after the burn-in period. It is noteworthy that at the end of the heating period, the tracer concentration error values are very small, compared to the errors obtained at the beginning of the Markov Chain generation, as already observed in Figs. 3 - 4. Thus, it can be seen that the tracer concentration profiles represented by the solid red lines occupy the same coordinates of the graph.

Therefore, based on the results presented, it is observed that the methodology used in this research work was efficient for the estimation of the longitudinal dispersion coefficient.

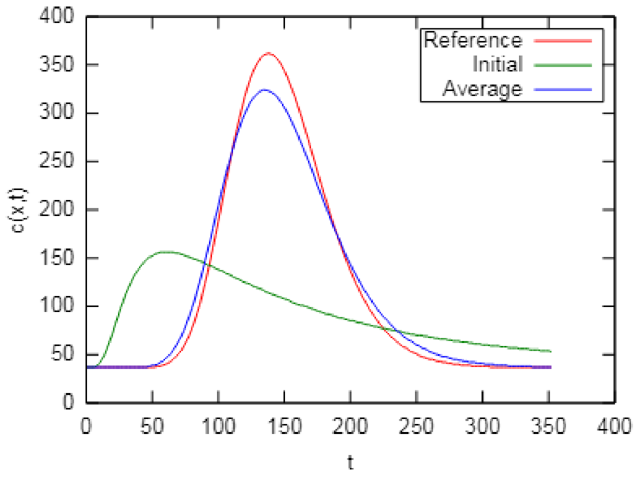

Fig. 7: Average of the last 50 samples before the burn-in period.

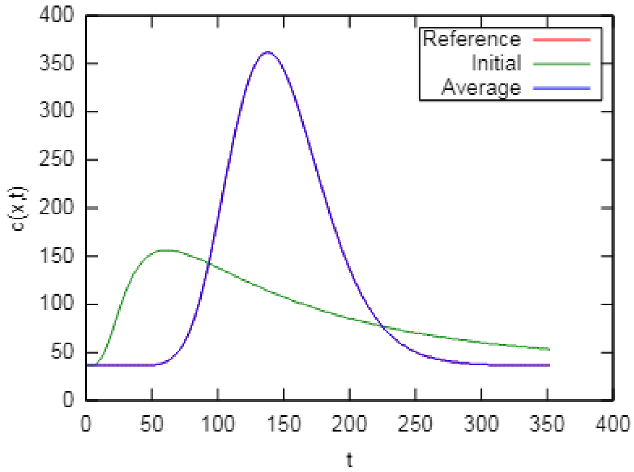

Fig. 8: Average of the first 50 samples after the burn-in period.

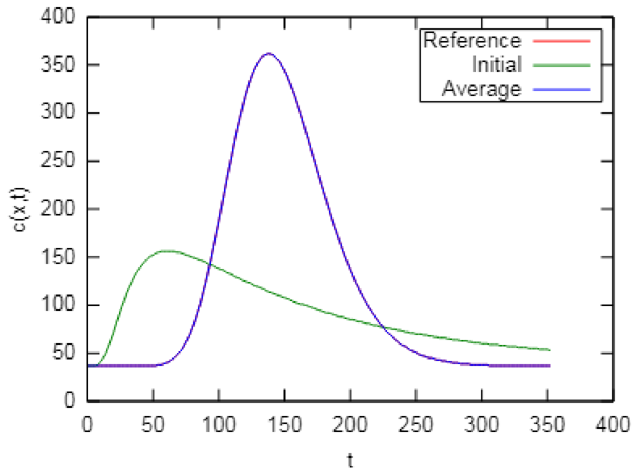

Fig. 9: Average of the first 150 samples after the burn-in period.

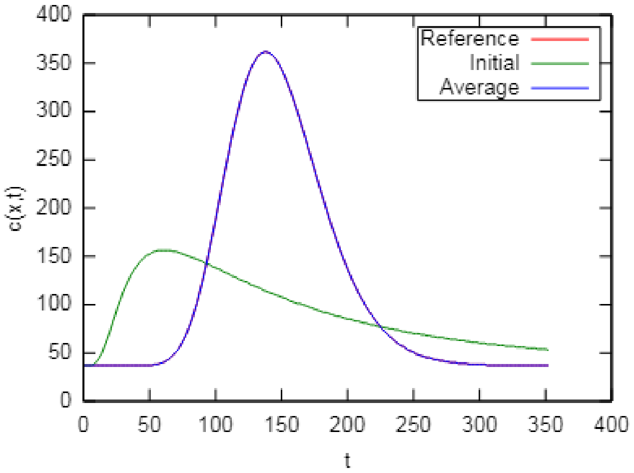

Fig. 10: Average of the first 250 samples after the burn-in period.

V. CONCLUSION

In this work, a statistical methodology was used to estimate the physical parameter longitudinal dispersion coefficient present in the tracer flow problem in natural rivers. This methodology consists of a Bayesian approach to formulate the inverse problem associated with the tracer transport problem, and an application of the Monte Carlo method via Markov Chains to solve the inverse problem formulated. Observing the numerical results obtained in this work, presented in Section IV, it can be stated that the MCMC method through the Metropolis-Hastings algorithm based on random walk generated a Markov Chain that converged to the equilibrium (or stationary) distribution, which in this case is the posterior distribution of interest. After the burn-in period, the accepted samples of the longitudinal dispersion coefficient were able to reduce the errors of the tracer concentration and, consequently, obtain better average simulated profiles of the tracer concentrations at the collection point. Thus, it can be said that the results achieved by the MCMC were quite expressive. This fact confirms the relevance of using statistical methodology to solve problems within the scope of behavioral prediction. The statistical tools used in this work were extremely efficient in estimating the values of the parameter of interest (longitudinal dispersion coefficient), which in turn can become a significant, respectable, useful and alternative resource for estimating parameters responsible for introducing uncertainties contained in the mathematical model that describes the physical process of tracer flow in natural rivers. However, it is also necessary that this methodology continues to be applied and tested in other types of problems, as well as the experimentation of new parameters and different formulations for the a priori distribution.

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