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PARAMETER ESTIMATION IN A SIMULATION OF TWO-DIMENSIONAL SEDIMENT TRANSPORT USING INTEGRAL TRANSFORM AND BAYESIAN INFERENCE

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Abstract. *In this work we develop an analytical-numerical hybrid solution through the Generalized Integral Transform technique (GITT) for solving a two-dimensional transient problem of transport of non-cohesive sediments. To accelerate the convergence of the hybrid solution analytical filtering was applied in order to homogenize the contours, and the equation was transformed into a coupled one-dimensional system of partial differential equations solved numerically employing Wolfram Mathematica 10. The results were compared with the solution obtained by NDSolve routine, indicating the feasibility of the solution of this problem by integral transform, which led to computational gains. For the identification of hydrodynamic parameters, we used Markov Chain Monte Carlo method, which showed results in agreement with the expected.*

Keywords: *Environmental Simulation, Sediment Transport, GITT, Inverse Problems.*

1. INTRODUCTION

Over the years there has been a growing concern about the increased concentration of pollutants in bodies of water, which originated mainly by disordered industrial and population growth. The movement of sediments represent one of the most common problems faced by the world population, and for this reason the knowledge and characterization of the sediment behavior in the water environment are essential for the protection of the environment, maintenance of navigation channels, construction hydraulic works, soil conservation and available water resources (Souza, 2010).

For a long time, the only available solution methods to solve advection-dispersion problems were through purely analytical techniques. The development of numerical large-scale application methods only recently emerged with the emergence of high performance computers. Numerical models are an important alternative for the qualitative and quantitative analysis of the hydrossedimentological processes that occur in water bodies, which with the advancement of computing has been gaining increasing interest in engineering projects. In the literature, several papers are presented with proposals for solutions for simplified versions of the advection-dispersion equation that simulates the transport of non-cohesive sediments (Sousa, 2009; Souza *et al.*, 2017; Souza, 2018). Among the different methodologies, the Generalized Integral Transform Technique (GITT) stands out because it is a hybrid method widely used in the solution of several problems by being able to combine the flexibility of the numerical methods with the robustness of the analytical methods (Cotta, 1993).

The use of hybrid methods has become even more interesting and viable with the evolution of programming systems. Along with this, the use of the Mathematica platform, a state-of-the-art software that brings together symbolic computing resources, enables the user to develop programs with automatic manipulation of analytical expressions. In addition to being recognized, both for its technical capacity and for its easy and sophisticated programming, this platform provides an integrated system, in continuous expansion with several programming libraries to be used in the most different areas of knowledge. In the literature, several papers are presented with proposals for solutions for simplified versions of the advection-dispersion equation that simulates the transport of non-cohesive sediments (Souza, 2018). The objective of this work is to get a hybrid solution of the 2D-vertical model of transport of non-cohesive sediments using GITT and the platform Wolfram Mathematica ® and estimate hydrodynamic and transport parameters present in this model by means of the Bayesian inference.

2. PROBLEM DESCRIPTION

The concentration of non-cohesive sediments for each granulometric class can be represented by the following advection-dispersion equation (Pinto *et al.*, 2012), and respective boundary and initial conditions (Rijn, 1986):

$$\frac{\partial C(x,z,t)}{\partial t} + U(z)\frac{\partial C(x,z,t)}{\partial x} - W_s\frac{\partial C(x,z,t)}{\partial z} = D_x\frac{\partial^2 C(x,z,t)}{\partial x^2} + D_z\frac{\partial^2 C(x,z,t)}{\partial z^2} \tag{1a}$$

$$C(0,z,t) = C_0, \qquad \frac{\partial C(L_x,z,t)}{\partial x} = 0, \quad 0 \le z \le L_z, \quad t > 0 \tag{1b}$$

$$W_s C(x,L_z,t) + D_z\frac{\partial C(x,L_z,t)}{\partial z} = 0, \qquad W_s C_a + D_z\frac{\partial C(x,0,t)}{\partial z} = D - E, \quad 0 \le x \le L_x, \quad t > 0 \tag{1c}$$

$$C(x,z,0) = C_1, \quad 0 \le x \le L_x, \quad 0 \le z \le L_z \tag{1d}$$

where $U(z) = u_*(8,5 + 5,75\log(u_* z/\nu))$ represents the velocity of the flow in the direction x, u_* is the friction velocity, ν is the kinematic viscosity, W_s is the velocity of fall of the sediment particle, D_x and D_z are the dispersion coefficients of the concentration in the directions x and z, respectively, L_x and L_z are the longitudinal and vertical lengths of the domain of interest, C_0 represents the continuous emission of a pollutant at the border, at the position $x = 0$, C_1 is the initial sediment concentration and C_a is a reference concentration in the flow bed under equilibrium conditions and D and E are the sediment deposition and erosion fluxes, respectively.

3. METHODOLOGY

3.1 Integral Transform

The solution of the problem is obtained by the GITT technique, by a partial transformation scheme, only in the vertical direction, resulting in a transformed problem formed by a system of one-dimensional partial differential equations.

The GITT technique can also be applied using a partial transformation methodology, when only one spatial coordinate is eliminated by integral transformation. This strategy uses more robust numerical methods and therefore can reduce the computational cost by algebraic manipulation and obtain more accurate solutions (Castelloes and Cotta, 2006; Cotta and Gerk, 1994). For the solution of the problem addressed in this chapter we considered a partial transformation scheme, only in the vertical direction, to eliminate the variable z. By the simplicity of the boundary conditions present in the problem (Cotta and Gerk, 1994), the spatial coordinate x is not eliminated by a second integral transformation. This procedure results in a transformed problem, thus formed by a coupled system of one-dimensional partial differential equations for the transformed potentials, which can be numerically treated to complete the solution procedure. This combination of solution methodologies is justified by providing an analytical and low cost computational representation for the expansion of auto-functions for the vertical coordinate together with a flexible and feasible numerical approach for the longitudinal behavior of the coupled transform potential (Castelloes *et al.*, 2007; Castelloes and Cotta, 2006).

In order to accelerate and optimize the convergence of the integral transformation technique, GITT, the problem was simplified with the application of the filter function $C_f(z) = \text{Exp}[-\frac{W_s}{D_z}z]/W_s$, used to homogenize the boundary conditions in z by the expression $C(x,z,t) = C_f(z) + C^*(x,z,t)$, where $C^*(x,z,t)$ is the solution of the homogeneous problem obtained through GITT. Consequently, the following associated eigenvalue problem is proposed:

$$D_z\frac{d^2\psi_i(z)}{dz^2} + \beta_i^2\psi_i(z) = 0 \tag{2a}$$

$$W_s C_a + D_z\frac{d\psi_i(0)}{dz} = 0 = W_s\psi_i(L_z) + D_z\frac{d\psi_i(L_z)}{dz} \tag{2b}$$

The problem presented allows us to define the following integral transformation pair:

$$\overline{C}_i(x,t) = \int_0^{L_z} \widetilde{\psi}_i(z) C^*(x,z,t)\,dz \qquad (transformed) \tag{3a}$$

$$C^*(x,z,t) = \sum_{i=1}^{\infty} \widetilde{\psi}_i(z)\overline{C}_i(x,t) \qquad (inverse) \tag{3b}$$

where $\widetilde{\psi}_i(z) = \dfrac{\psi_i(z)}{\sqrt{N_i}}$ are the normalized auto-functions with $N_i = \int_0^{L_z} \widetilde{\psi}(z)^2 dz$.

The Equation (1a) is transformed by the operator $\int_0^{L_z} \widetilde{\psi}_i(z)(.)dz$ which is applied on both sides of the equation to obtain the following transformed problem, Eq. (4a), with initial and boundary conditions, Eq. (4b), given by:

$$\frac{\partial \overline{C_i}(x,t)}{\partial t} + \sum_{j=1}^{\infty} \frac{d\overline{C}_j(x,t)}{dx} \int_0^{L_z} \widetilde{\psi}_i(z)\widetilde{\psi_j}(z)U(z)dz - W_s \sum_{j=1}^{\infty} \overline{C}_j(x,t) \int_0^{L_z} \widetilde{\psi}_i(z)\frac{d\widetilde{\psi_j}(z)}{dz}dz = D_x \frac{\partial^2 \overline{C_i}(x,t)}{\partial x^2} - \beta_i^2 \overline{C_i}(x,t) \tag{4a}$$

$$\overline{C_i}(x,0) = \int_0^{L_z} \widetilde{\psi}_i(z)(C_1 - C_f(z))dz, \qquad \overline{C_i}(0,t) = \int_0^{L_z} \widetilde{\psi}_i(z)(C_0 - C_f(z))dz, \qquad \frac{\partial \overline{C_i}(L_x,t)}{\partial x} = 0 \tag{4b}$$

The above system is solved numerically for the transformed potentials $\overline{C_i}(x,t)$, so that the inversion formula, Eq. (3b), can be used to obtain the solution for filtered potential, $C^*(x,z,t)$.

The implemented solution requires the knowledge of parameters that are difficult to measure, such as the longitudinal (D_x) and vertical (D_z) dispersion coefficients, whose values are usually obtained through field experiments using the plotter technique. The difficulty of manipulating the material used as tracer is one of the disadvantages of this technique, besides a possible contamination of the environment. A very efficient alternative for estimation of these two dispersive parameters and sediment particle settling velocity (W_s) and friction velocity near the bottom of the stream (u_*) can be obtained by analyzing the inverse problem.

3.2 Inverse Problem

Evidently, the deterministic models made a great contribution to the understanding of the dynamic behavior of a system. However, they fail to circumvent the uncertainties present in a model and end up being insufficient in the decisionmaking stages. Measurement errors are not the only factors that contribute to these uncertainties during the inverse problem estimation process. Other factors, such as the formulation of the problem and the boundary conditions and the technique used to optimize the unknown parameter vector, may affect the final solution and present an inconsistent result in the inverse analysis, even if at first all the variables seem to be well defined. In parallel, there is a diversity of physical phenomena that can be described through stochastic processes due to their ability to simulate noise and uncertainties present in experimental observations.

In the inverse analysis, which consists of obtaining estimates for the parameters D_x, D_z, u_* and W_s, present in Eqs. (1a)-(1d), Bayesian Inference was used. The advantages of this approach are the possibility of including a priori information and incorporating it into a formal decision context, as well as the explicit treatment of uncertainties and the ability to assimilate new information in adaptive contexts (Graham, 2014).

Considering the experimental data supposed to be acquired in a fixed time interval and normally distributed measurement errors with zero mean and constant standard deviation, the solution of the inverse problem of parameter estimation by the Bayesian approach here is to obtain the posterior probability ($P_{post}(\boldsymbol{\beta}|\boldsymbol{Z}_e)$), with the use of Bayes' theorem, such that:

$$P_{post}(\boldsymbol{\beta}|\boldsymbol{Z}_e) = P(\boldsymbol{Z}_e|\boldsymbol{\beta})P_{pr}(\boldsymbol{\beta})/P(\boldsymbol{Z}_e) \tag{5}$$

where $P_{pr}(\boldsymbol{\beta})$ is the priori probability, $P(\boldsymbol{Z}_e)$ is the marginal probability and $P(\boldsymbol{Z}_e|\boldsymbol{\beta})$ is the likelihood obtained by Eq. (6) which describes the probability of finding the experimental data $\boldsymbol{Z}_e$, knowing the actual and unknown response of the physical problem ($\boldsymbol{Z}(\boldsymbol{\beta})$) and the variance ($\boldsymbol{V}$) of the experimental data (Schwaab and Pinto, 2007):

$$P(\boldsymbol{Z}_e|\boldsymbol{\beta}) = \frac{1}{\sqrt{det\boldsymbol{V}(2\pi)^{n_e}}} \exp\left[-\frac{1}{2}(\boldsymbol{Z}_e - \boldsymbol{Z}^m)^T \boldsymbol{V}^{-1}(\boldsymbol{Z}_e - \boldsymbol{Z}^m)\right] \tag{6}$$

where n_e represents the number of experimental data considered in the problem.

A priori information can not always be represented by a normal or even uniform distribution, which makes it very difficult to obtain a posteriori probability distribution. In these cases, it is necessary to use sampling techniques to simulate the posterior distribution samples and to infer measures of central tendency and dispersion of this distribution (Kaipio and Somersalo, 2006). Among these sampling techniques, the Markov Chain Monte Carlo method (MCMC) stands out. The essential idea of MCMC is to simulate a random sequence of the posterior distribution of each parameter of interest of the inverse problem convergent to a stationary distribution.

4. RESULTS

For the analysis and verification of the effectiveness of the methods of solution of the direct and inverse problem was considered the hypothetical case of a channel with dimensions of 200 m length by 1 m depth, with a continuous and constant flow of $C_0 = 50mg/l$ entering the domain in $x = 0$. In addition, the following values were used to solve the direct problem: $C_1 = 50mg/l$, $C_a = 100mg/l$, $D - E = 0,1kg/m^2s$, $W_s = 0,013m/s$, $u_* = 0,15m/s$, $D_x = 0,25m^2/s$ and $D_z = 0,006m^2/s$.

The convergence behavior of the solution as a function of the series truncation (N) - Eq. (3b) - is shown in Table 1-4. It is observed that the results converged to at least two significant digits, demonstrating that only 5 terms of the series are enough to obtain a good convergence of the model.

Table 1. Convergence analysis of the solution in relation to the order of truncation ($z = 0,5$ m).

x (m)	N=2	N=5	N=10	N=20	N=50	N=100
			$t = 50$ s			
0	47,939841	51,307159	49,558268	49,901118	50,024095	49,996225
40	40,157284	39,825171	39,967085	39,990508	39,991084	39,991274
80	40,018214	39,658897	39,797702	39,820180	39,820842	39,820954
120	40,018214	39,658597	39,797816	39,820180	39,820842	39,820954
160	40,018214	39,658591	39,797815	39,820180	39,820842	39,820954
200	40,018214	39,658591	39,797815	39,820180	39,820842	39,820954

Table 2. Convergence analysis of the solution in relation to the order of truncation ($z = 0,5$ m).

x (m)	N=2	N=5	N=10	N=20	N=50	N=100
			$t = 100$ s			
0	47,939841	51,307159	49,558268	49,901118	50,024095	49,996225
40	40,020650	40,032548	40,087023	40,099034	40,099979	40,100056
80	33,827856	33,783115	33,804730	33,809621	33,809840	33,809848
120	32,040868	32,003207	32,011488	32,013176	32,013237	32,013302
160	31,835282	31,815674	31,819277	31,819709	31,819718	31,819751
200	31,834974	31,815374	31,818993	31,819424	31,819429	31,819457

Table 3. Convergence analysis of the solution in relation to the order of truncation ($x = 100$ m).

z (m)	N=2	N=5	N=10	N=20	N=50	N=100
			$t = 50$ s			
0	103,22075	102,95371	103,14173	103,17629	103,17748	103,17779
0,2	70,386478	70,095591	70,251324	70,278406	70,279383	70,279618
0,4	48,294629	47,954539	48,089713	48,117588	48,118407	48,118562
0,6	33,123089	32,755102	32,890390	32,908253	32,908868	32,908941
0,8	22,496013	22,154797	22,237880	22,254420	22,254801	22,254818
1,0	14,897526	14,641833	14,678076	14,683198	14,683253	14,683225

In all subsequent simulations, five terms were used in the serial expansion of the solution of the problem, which was sufficient to obtain the desired precision in at least two digits of convergence to the concentration field. The Fig. 1 show the temporal evolution of sediment concentrations by GITT in the central region of the flow.

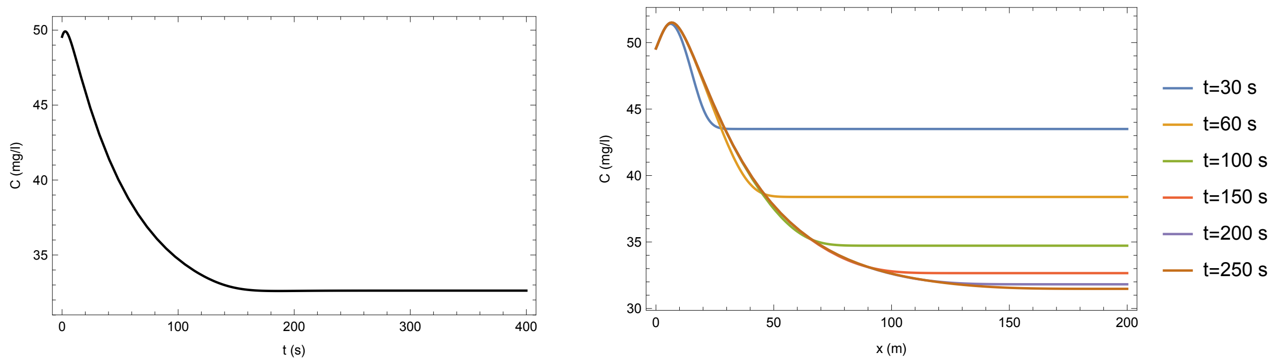
After 200 seconds of simulation, the permanent sediment transport regime is observed. The Fig. 2 show the solution of the direct problem by GITT and the Mathematica's NDSolve routine for the concentration of non-cohesive sediments along the domain of interest.

In order to compare the two methods of solution, we considered the relative error given by the expression:

$$E_r = \frac{|C(Gitt) - C(NDSolve)|}{C_a} \tag{7}$$

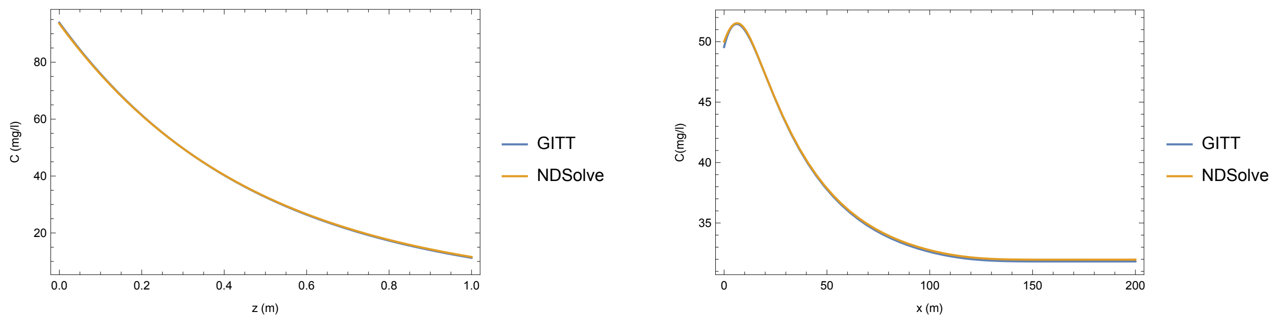
Table 4. Convergence analysis of the solution in relation to the order of truncation ($x = 100$ m).

z (m)	N=2	N=5	N=10	N=20	N=50	N=100
			$t = 100$ s			
0	97,086383	96,901276	96,966154	96,977399	96,977787	96,977803
0,2	64,410352	64,220646	64,269194	64,276983	64,277280	64,277292
0,4	42,780342	42,599079	42,641526	42,650652	42,650923	42,650958
0,6	28,338870	28,207303	28,253591	28,258879	28,259106	28,259157
0,8	18,660722	18,599136	18,623001	18,628463	18,628627	18,628678
1	12,176320	12,152168	12,159044	12,160152	12,160213	12,160242



(a) x = 100 m and z = 0,5 m (b) z = 0,5 m

Figure 1. Temporal distribution of sediment concentration.



(a) z (m) (b) x (m)

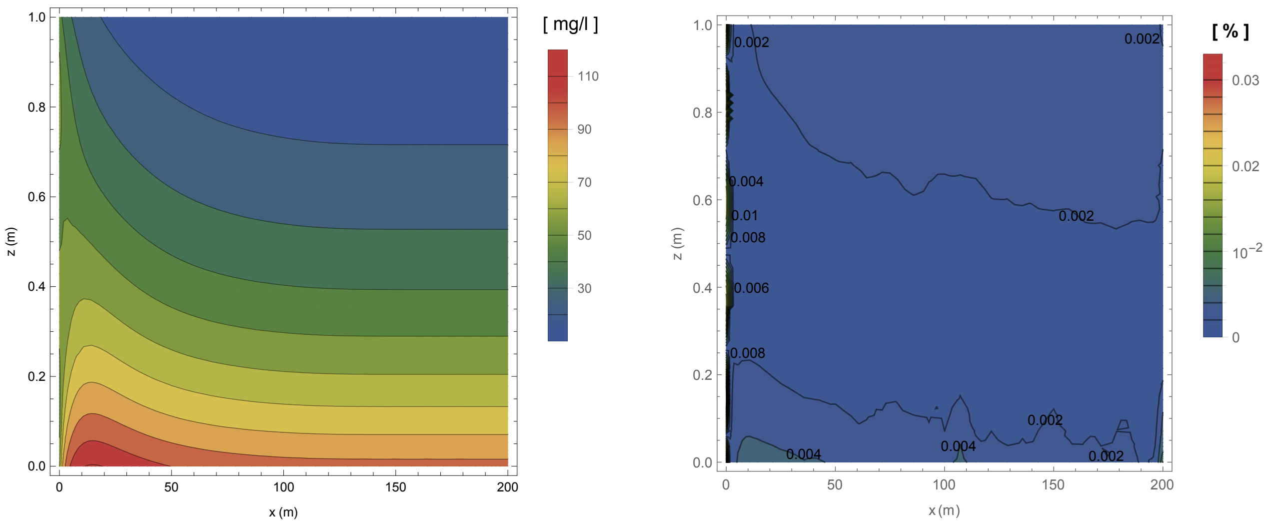
Figure 2. Vertical distribution of sediment concentration at time t = 200 s.

The spacial distribution of suspended sediment concentration in steady state after 200 segundos of simulation are presented in Fig. 3.

The results were found to be similar with an error of up to 4% of the background reference concentration. The solutions by GITT and the NDSolve routine had a computational cost of 0,30 seconds and 11,89 seconds, respectively. With GITT, the computational gain was high, generally being on the order of 40 times faster than NDSolve Routine, demonstrating the adequacy of the use of this technique for the analysis of the inverse problem.

For the solution of the inverse problem with the MCMC method we have considered a non-informative a priori for D_z and W_s from a uniform distribution. Due to the difficulty in estimating the parameters D_x and u_*, a priori information was considered for these two parameters according to a normal distribution with means of, respectively, 0,25 m^2/s and 0,15 m/s, and standard deviation of 20% of each mean, with level of noise of 5% of the initial concentration. As there were no real experimental data available for the inverse analysis, synthetic data were obtained at the position x = 100 m and z = 0,5 m. To this experimental information were added random noise according to a normal distribution with mean zero and known standard deviation (σ_e), as presented $C_{ei} = C_i(\beta^{exact}) + \sigma_i,\sigma_i \sim N(0, \sigma_e)$, $i = 1, ..., N_e$. The data were generated with $\sigma_e = 2,5$ mg/l of noise during 150 s of simulation of the direct problem with the exact values of the parameters.

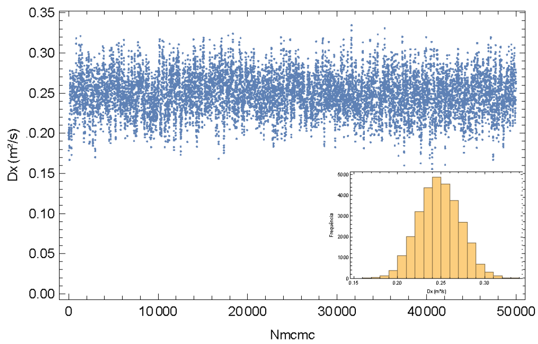
The results of the MCMC are presented in Fig.4, where the histograms and the convergence of the Markov chains are observed for the mean values $D_x = 0,24981 m^2/s$, $D_z = 0,00591 m^2/s$, $u_* = 0,15426 m/s$ and $W_s = 0,01280 m/s$, considering a chain of 50 000 states and heating of 10 000 states. The parameters of interest were estimated through the Metropolis-Hastings algorithm, accepting or rejecting at each iteration the candidate parameter vector. It is observed from



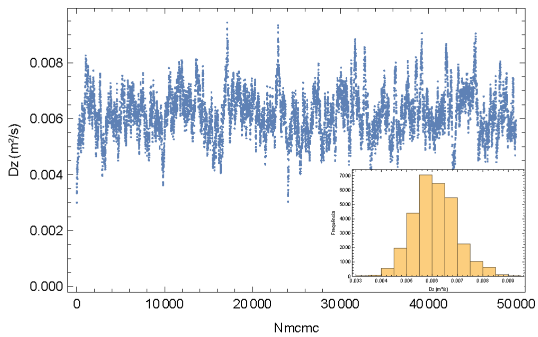
(a) GITT (N=5) (b) Relative Error (E_r)

Figure 3. Spatial distribution of sediment concentration at time t = 200 s.

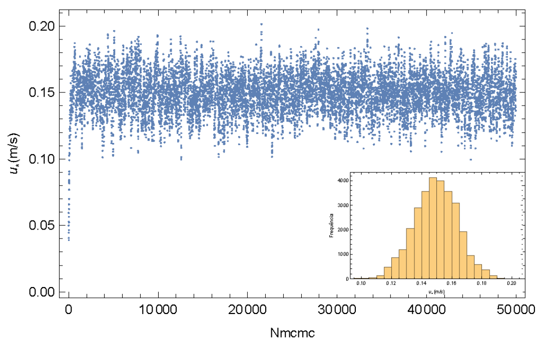
the figures that the convergence of the chains obtained by the MCMC occurred already in the initial stages of the iterative process.



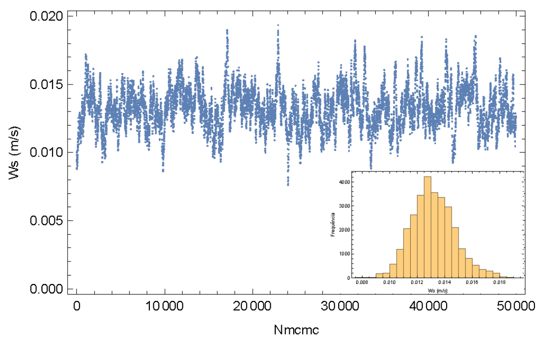
(a) D_x



(b) D_z



(c) u_*



(d) W_s

Figure 4. Evolution of Markov Chains.

Considering a noise of $\sigma_e = 2,5mg/l$, it is observed that MCMC demonstrated efficiency to reach a steady state for all parameters of interest, with a 95% confidence level.

In order to facilitate the comparison between the results found by the MCMC, Table 5 presents the main statistical properties of the parameters of interest with mean values, standard deviation, coefficients of variation, RMS and confidence intervals with of 95% confidence. By analyzing the data from the Table 5, it is verified that all the parameters were shown within the respective confidence intervals. In addition, a relatively low RMS value was obtained for parameter adjustment.

Of the 40000 Markov chain samples considered in the statistical analysis were accepted 12568 states. The efficiency of the MCMC and the good agreement between the exact and calculated parameters are proven by the low RMS value

Table 5. Statistical properties of the parameters using noise of σ_e = 2,5 mg/l

Parameter	Exact	μ	σ	$\sigma/\mu(\%)$	I.C. (95%)
D_x	0,25	0,249819	0,024735	10,346	[0,201042;0,297235]
D_z	0,006	0,005912	0,000614	10,385	[0,004796;0,007128]
u_*	0,15	0,154260	0,012655	8,203	[0,129280;0,177654]
W_s	0,013	0,012806	0,00116	9,058	[0,010677;0,015115]
Acceptance Rate (%)	31,42				
RMS (mg/l)	0,00810335				

obtained.

All calculated parameters were included in the confidence intervals. Considering the mean values of the parameters obtained by the MCMC and the synthetic experimental data, the Fig. 5 show the good quality of the agreement.

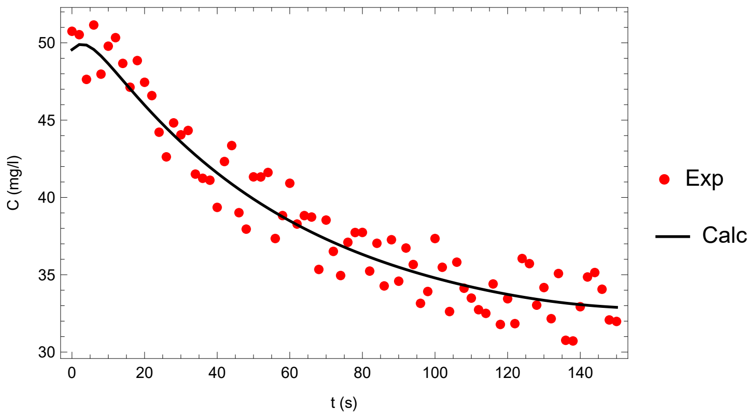


Figure 5. Comparison between the solution of the inverse problem and the experimental data.

In general and immediate, the good agreement between the estimated values of the dispersive and transport properties is observed, showing a very small variation, which was expected, demonstrating that the adhesion between the experimental and theoretical curves is consistent. The estimates for the parameters involved in the model were very accurate, which allows to describe the sediment concentration profile, as well as the temporal and spatial evolution of the concentrations in the entire domain of interest.

5. CONCLUSIONS

The methodology used here allowed, through the inverse problem, to estimate hydrodynamic and transport parameters, in general, difficult to measure, consequently making possible the observation of expected behaviors for the concentration of non-cohesive sediments in natural water bodies.

The use of the GITT technique in the solution of the proposed problem proved plausible and rapid, as it was desirable for the viability of the solution of the inverse problem. The Markov Chain Monte Carlo Method proved to be effective in solving the problem of identifying dispersive and transport parameters with an average execution time of approximately 9 hours.

The use of hybrid strategies through the GITT technique demonstrated a great potential for use in the solution of inverse problems with several possibilities of application. Obviously for models with greater complexity the use of the technique presents greater difficulty but, when properly implemented, provides good approximations to the solution of the problem.

For future work, it is recommended to apply the MCMC to estimate the longitudinal velocity present in the advective term, as well as to set smooth functions that describe the fluxes present in the boundary conditions, especially on the surface and the bottom of the flow. Another important recommendation is the application of methodologies that allow the reduction of the computational cost of the inverse problem.

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