WARNING SYSTEM BASED ON THEORETICAL-EXPERIMENTAL STUDY OF DISPERSION OF SOLUBLE POLLUTANTS IN RIVERS¹

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ABSTRACT: Information about capacity of transport and dispersion of soluble pollutants in natural streams are important in the management of water resources, especially in planning preventive measures to minimize the problems caused by accidental or intentional waste, in public health and economic activities that depend on the use of water. Considering this importance, this study aimed to develop a warning system for rivers, based on experimental techniques using tracers and analytical equations of one-dimensional transport of soluble pollutants conservative, to subsidizing the decision-making in the management of water resources. The system was development in JAVA programming language and MySQL database can predict the travel time of pollutants clouds from a point of eviction and graphically displays the temporal distribution of concentrations of passage clouds, in a particular location, downstream from the point of its launch.

KEYWORDS: longitudinal dispersion, water pollution, computational modeling.

SISTEMA DE ALERTA COM BASE EM ESTUDO TEÓRICO-EXPERIMENTAL DE DISPERSÃO DE POLUENTES SOLÚVEIS EM RIOS

RESUMO: Informações sobre a capacidade de transporte e dispersão de poluentes solúveis em cursos de água naturais são importantes no gerenciamento dos recursos hídricos, principalmente no planejamento preventivo de medidas que visem a minimizar problemas à saúde pública e às atividades econômicas que dependem do uso da água, ocasionados por despejos acidentais ou intencionais. Considerando tal importância, este trabalho teve como objetivo desenvolver um sistema de alerta para rios, com base em resultados experimentais, utilizando técnicas de traçadores e equações analíticas de transporte unidimensional de poluentes solúveis conservativos, visando a subsidiar a tomada de decisão no gerenciamento dos recursos hídricos. O sistema desenvolvido em linguagem de programação JAVA e banco de dados MySQL permite prever o tempo de percurso da nuvem de poluentes a partir de um ponto de despejo de um poluente e apresenta, graficamente, a distribuição temporal de concentrações da passagem da nuvem, em um determinado local, à jusante do ponto do seu lançamento.

PALAVRAS-CHAVE: dispersão longitudinal, poluição hídrica, modelagem computacional.

INTRODUCTION

In Brazil, the situation of water pollution has worsened due to increased urban and industrial pollution discharges, inappropriate land use and agricultural inputs (MORAES & PAULA JÚNIOR, 2004; DAGA et al., 2007), erosion (PRUSKI, 2006), deforestation and mining (MACHADO et al., 2008). In this context, the increased transport of sediment, and organic and chemistry contamination in the water are particularly notable in terms of degradation of water resources.

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This critical situation required careful analysis during the implementation of new projects, when there is effluent disposal into rivers (MACHADO et al., 2008).

Thus, the quantification of parameters related to transport and dispersion of soluble pollutants into natural water streams is of great importance in the planning and management of water resources, especially in accidental or intentional cases, when it is necessary to warn the populations located downstream of the discharge site about the risks they are subjected when taking water from watercourses to meet their basic needs.

The warning system allows predicting the time course of the pollution cloud from an instantaneous or continuous discharge of an effluent and the graphical representation of the concentration distribution in time of the cloud passing a particular location downstream of the discharge site.

The complexity and diversity of natural water flows make a purely theoretical approach difficult to predict longitudinal dispersion parameters (D_L). Experiments with tracers are an appropriate approach to determine the longitudinal dispersion coefficient, as it allows to reliably simulate the movement and dispersion of the solute, implicitly taking into account all peculiarities and characteristics of transport and dispersion of the flow, according to studies reported by SOARES et al. (2010) and RIBEIRO (2007).

Another method used to predict D_L is to employ empirical equations that allow estimation based on flow-related parameters (RIBEIRO et al., 2010 and DEVENS et al., 2006).

It is known that there currently is a growing need of tools to assist in the planning and management of problems related to management of water resources (MACHADO et al., 2008). Thus, the main objective of this study was to develop a warning system for rivers, based on experimental results using tracer techniques and analytical equations of one-dimensional transport of conservative soluble pollutants.

MATERIAL AND METHODS

The study area where field studies were carried out to determine the coefficient of longitudinal dispersion comprises the Pomba River watershed, located in the Zona da Mata Mineira, an affluent of the Paraíba do Sul River (Figure 1).



FIGURE 1. Location of Pomba river watershed.

Four sections of the Pomba River watershed, comprising a 36-km stretch, were monitored. The monitored stretch includes the municipalities of Astolfo Dutra (PMB1), Dona Euzébia (PMB2), Sinimbú (PMB3) e Cataguases (PMB4), as shown in Figure 2. Two experiments were conducted to determine "on site" the characteristics of transport and dispersion of the Pomba River. The first experiment was performed in 27-28 May 2006, and the second one, in April 14-15, 2007, in order to characterize the behavior of the river at different times.



FIGURE 2. Monitoring sections of the Pomba River.

Table 1 shows the main features of the monitoring sections of the Pomba River.

Monitored Sections	Distance ^{*1} (km)	Coordinates	Description	
Disaharaa	0.0	21°18'39.95" S	Downstream U.H.E. Ivam	
Discharge		42°54'14.68" W	Botelho - Pomba River	
PMB_1* ²	6.0	21°18' 34.86" S	Bridge over Pomba river in the	
		42°51' 43.21" W	municipality of Astolfo Dutra	
PMB_2	13.0	21°19' 6.77" S	Bridge over Pomba river in the	
		42°48'43.28" W	municipality of Dona Euzébia	
PMB_3	22.0	21°20' 55.12" S	- Bridge over Pomba river in Sinimbu	
		42°44'53.58" W		
PMB_4	36.0	21°23'23.62" S	Bridge over Pomba river in the	
		42°42'6.68" W	municipality of Cataguases	

TABLE 1. Characteristics of the monitoring sections of the Pomba River.

*¹ Distance in relation to the point where the tracer was discharged. *² monitoring point in the Pomba River.

Field and laboratory work to determine the D_L

The fluorescent tracers Uranina or sodium fluorescein (Acid Yellow 73, color index 45350) and Amidorhodamine G Extra (Acid Red 52, color index 45220) were used in the field experiments. These tracers have the property of emitting light (fluorescence) at a certain wavelength range when light of another particular (shorter) wavelength, for which the tracer is sensitive, is beamed on the compound (excitement).

It was chosen to perform an instantaneous tracer discharge, as shown in Figure 3.



FIGURE 3. Instantaneous discharge of tracers Amidorhodamine G Extra and Uranina in the Pomba River, downstream of the Ivan Botelho hydroelectric power plant.

Dislocation monitoring of the tracer cloud was conducted from fixed coordinates (monitoring sections), over bridges, featuring an Euler monitoring type. During the field experiments, a Turner fluorometer Model 10, given by the Tracer Laboratory at COPPE/UFRJ, was used to detect "on site" tracer concentrations in the range between 0.5 and 1.0 ppb, to evaluate the displacement of the tracer cloud. Approximately 400 water samples (approximate 100 mL volume each) were collected in each experiment, with approximately 100 samples in each section (PMB1, PMB2, and PMB3 PMB4) in regular time intervals, ranging from 10 to 30 minutes, according to the hydrodynamic development downstream of the tracer cloud.

The laboratory work consisted of preparing standard solution concentrations of 0.1; 0.2; 0.5; 1.0; 2.0; 5.0 and 10.0 μ g L⁻¹ for calibration curves (water was used as diluting agent, being 1 μ g L⁻¹ equivalent to 1 ppb), using 20 liters of water collected from the Pomba river as solvent. Fluorimetry measurements of standard dilutions allowed the establishment of calibration curves to linearly correlate with the fluorescence patterns with their concentrations. From these curves, it was obtained concentration values for each sample collected in the field.

One-dimension mass transport equation for D_L determination

The determination of the longitudinal dispersion coefficient (D_L) , from the tracer experiments is based on the equation of one-dimensional mass transport (advection and dispersion) of conservative constituents (Equation 1):

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = D_L \frac{\partial^2 C}{\partial x^2}$$
(1)

where,

C - average concentration of soluble substance, ML^{-3} ;

t - time, T;

U - average flow speed, LT^{-1} ;

 D_L - longitudinal dispersion coefficient in the direction of flow, L^2T^{-1} ;

x - distance traveled by the pollutant, L;

$$U \frac{\partial C}{\partial x}$$
 - advective transport, MT⁻¹L⁻³, and
 $D_L \frac{\partial^2 C}{\partial x^2}$ - dispersive transport of pollutant, MT⁻¹L⁻³.

Solution of the one-dimensional dispersion equation can be obtained from considerations about the initial and adjacent conditions, as shown below.

Considering the initial condition equivalent to an instantaneous discharge uniformly distributed over the cross section, i.e., an amount of mass M in a concentrated infinitely small space at time t = 0 and the origin of the x-axis, we have (Eq. 2 and 3):

$$C(0, t_0) = M \delta(x)$$
⁽²⁾

$$C (x \neq 0, t_0) = 0$$
 (3)

where, $\delta(x)$ equals to Dirac delta function and M is the constituent mass (kg).

And for the surrounding conditions, considering the equations (4) e (5):

C
$$(-\infty, t) = 0$$
 (4)
C $(+\infty, t) = 0$ (5)

The solution is a Fick's model, also known as the Taylor's model or method of adjustment, as shown in Equation (6):

$$C(x, t) = \frac{M}{A\sqrt{(4\pi D_{L}t)}} \exp \frac{-(x - Ut)^{2}}{4D_{L}t}$$
(6)

where,

C - concentration of constituent or pollutant, ML^{-3} ;

M - mass of constituent discharged, M;

A - area of cross-section, L^2 ;

 D_L - longitudinal dispersion coefficient, L^2T^{-1} ;

U - flow rate, LT^{-1} , and

X e t - spatial (L) and temporal (T), variable, respectively.

Figure 4 illustrates the effects of physical processes of diffusion and advection, where the advective flow is responsible for the displacement Δx and diffusive flow causes the dispersal of soluble substances in the flow.



FIGURE 4.Illustration of mass transport of a substance discharged instantaneously in a uniform and laminar flow by advection and diffusion mechanisms.

DEVENS et al. (2006) reported that the convolution method has the advantage of being independent of the form of discharge of the soluble constituent.

Development of the warning system

Information regarding the hydrodynamic parameters (speed and longitudinal dispersion) obtained in field experiments was stored in a database, thus allowing to develop a warning system.

For the construction of the graphical interface, it was used JAVA programming language, and to store information on water samples collected in the Pomba River, as well as internally generated data in the model, it was used the MySQL database.

Methods of adjustment and convolution were respectively used to predict the transport and dispersion of pollutants from immediate and continuous pollutant source. In this case, D_L is no longer unknown and becomes an important input parameter to feed the predictive models of pollutant transport.

It is noteworthy that in the case of a continuous release, for example of an industry, one must provide flow values of the released effluent over time, and the concentration of the substance discharged in each time point, to allow calculating the concentration of the first occurrence or the mixture in the river, by using Equation (7).

$$C_{\rm M} = \frac{C_{\rm R} \ Q + C_{\rm E} \ Q_{\rm E}}{Q + Q_{\rm E}} \tag{7}$$

where,

 C_M - concentration of first occurrence or the mixture, ML⁻³; C_R - concentration of the substance in the river, ML⁻³; Q - river flow rate, L³T⁻¹; C_E - substance concentration in the effluent, ML⁻³, and Q_E - effluent flow rate, L³T⁻¹.

The convolution method (Equations 8 and 9) uses the principle of superposition of effects to generate, through a convolution integral of the distribution upstream, the concentration distribution in a section downstream.

$$C(x_{2},t) = \int_{\tau_{i}}^{\tau_{f}} \frac{m(x_{1},\tau) U}{2 Q_{2} \sqrt{\pi D_{L}(t-\tau)}} exp \left\{ -\frac{\left[\Delta x - U(t-\tau)\right]^{2}}{4 D_{L}(t-\tau)} \right\} d\tau$$
(8)

where,

- $C(x_2, t)$ tracer (or contaminant) concentration in the downstream section at time t, composed by the superposition of the responses of units discretization of instant mass, from the distribution curve concentrations upstream, ML⁻³;
- m (x_1, τ) unit of tracer (or contaminant) mass measured upstream, by slicing of the area under the curve in a time τ , M;
- τ times corresponding to the passage of the concentration distribution curve of the upstream section, T;
- τ_i instant of time corresponding to the beginning of the concentration distribution curve of the upstream section, T;
- τ_f instant of time corresponding to the end of the concentration distribution curve of the upstream section, T;
- t instant of time corresponding to the passing of the concentration distribution curve of the upstream section, T;
- Q_i flow rate of the river in the section considered, where i can be either 1 or 2. When i equals to 1, it represents the upstream section; and when i equals 2, it represents the downstream section, L^3T^{-1} , and
- Δx distance between the upstream and downstream sections of the stream, L.

The calculation of each instant mass obtained by slicing of the concentration distribution curve upstream is shown in Equation (9).

$$m(x_{1},\tau) = \left[\frac{\left[C(x_{1},\tau+1)+C(x_{1},\tau)\right]\left[(\tau+1)-\tau\right]}{2}\right]Q_{1}$$
(9)

Figure 5 illustrates the mass transport of a soluble substance continuously discharged over time, using the convolution method for downstream discharge mass transfer.

The system also allows the automatic determination of the average speed and dispersal capacity of the river (D_L) in the studied section, or interactively, from the adjustment of the Taylor's Fick model or the convolution of concentration values of the travel curve experimentally determined in the field with the use of tracer.



FIGURE 5. Illustration of mass transport of a soluble substance discharged continuously by advection and diffusion mechanisms.

In the alternative of automatic adjustment, the mean square error (RMSE) is used to automatically determine the best combination of speed values U and D_L , so that the mean square error between the experimentally measured values and the values adjusted by the models are the smallest possible.

$$EMQ = \frac{1}{N} \sum_{i=1}^{N} \left[E_i - O_i \right]^2$$
(10)

where,

 E_i - estimated values for the ith event; O_i - observed values for the ith event, and N - number of events.

In the option of manual adjustment, the coefficient of dispersion and average travel speed of the section under study are provided interactively by the user until the adjustment of the model visually best fit the measured values.

Figure 6 shows the flow chart of system operation.



FIGURE 6. Flow chart of the system.

RESULTS AND DISCUSSION

The warning system developed herein enables working with two distinct modules. The first module refers to the calculation of the longitudinal dispersion coefficient from experimental field results or by means of empirical formulas, being particularly important for calibrating water quality models that use this parameter in its structure. The second module includes the warning system itself, which can simulate the effect of an accidental or intentional, instantaneous or continuous, discharge in a downstream section of interest, serving as an important mechanism to alert citizens that use water resources in situations of discharge of potentially toxic substances.

Module I system - calculating D_L

Figure 7 illustrates the screen of the system used for registration of experimental data from a campaign of tracers in a monitoring section, in order to obtain the longitudinal dispersion coefficient.

Ø Disessa ős	
Cálculo do DI Sistema de Alerta	
Experimental Entrada de dados	Bio
Fórmula Reta de calibração	Secão
Iniecão instantânea	l Vertical
Convolução	Tracador
	Campanha
	Características da secão
	Coleta
	A Cadastro das características da secão
	Pio Bio Domha
	Vazão (m ³ /s) Velocidade (m/s)
	Distância co porte de iniceão (km)
	Salvar Editar Excluir Buscar 07/06/2006 🔻

FIGURE 7. Data registration (flow rate, mean speed, distance to the local discharge) relative to monitoring sections in a tracer experiment.

After filling in the information with data relative to a field experiment, the system allows to determine the parameters of longitudinal dispersion and average travel speed, for each monitoring section, automatically or interactively.

Figure 8 illustrates an automatic determination of the longitudinal dispersion coefficient and mean speed of the flow.



FIGURE 8. D_L and U calculation: (a) considering an instantaneous pollutant discharge (Adjustment Method); (b) considering a continuous pollutant discharge in the water flow (Convolution Method).

Still in the first module of the program it is possible to determine the longitudinal dispersion coefficient by means of empirical formulas, as presented in Figure 9.

🕼 Dispersão	
Cálculo do DL Sistema de Alerta	
Experimental >	
Formula	
🗟 Cálculo da dispersão por fórmula	
H = Profundidade (m)	Ribeiro (2007)
Rh = Raio Hidráulico (m)	
g = Aceleração da gravidade (m/s ³)	
So = Declividade do Leito (m/s)	$D_{T} = 7.326 (u_{*})^{0.303} (H)^{1.316} (B)^{0.445} (U)^{1.458}$
B = Largura do rio/canal (m)	
U = Velocidade (m/s)	
u* = Velocidade de cisalhamento (m/s)	
Fórmula proposta Ribeiro (2007)	
Dispersão Longitudinal (m²/s)	
	Calcular

FIGURE 9. D_L calculation through empirical equations (RIBEIRO et al., 2010).

It is worth noting that 13 different empirical formulas can be chosen to calculate the value of D_L by opening the box next to the "proposed formula". Once the formula is chosen, its image appears on the right side of the screen of the system, as shown in Figure 9.

Module II of the system - warning system

The warning system module allows simulating the effects of an accidental or intentional discharge of a soluble substance in a downstream section (defined by their distance from the discharge site).

The user must first choose between two types of discharge, instantaneous or continuous. Once it is defined, the user should enter the hydrogeometric data of the river (flow rate, average speed of flow and the longitudinal dispersion coefficient) into the system as well as the discharge characteristics, including the mass instantaneously discharged, in the case of instant discharge, or the effluent distribution concentrations over time, in case of continuous discharge, and local information, such as: discharging site, substance, time and date of discharge, and the distance from the section of interest to the discharging site.

The system was tested based on data acquired from experiments performed by SOARES et al. (2010) and RIBEIRO (2007).

It is noteworthy that for the experimental data used to compare against the data calculated by the warning system, considering the case of instantaneous discharge of pollutants, the results consisted of the travel of the maximum concentration of the constituent cloud in one section of the stream of interest, downstream of the release, and their respective travel time, as shown in Table 2.

Author/ Experiment - Section	Discharged Mass M (kg) / Calculated D_L "on site" (m ² s ⁻¹)	Flow rate Q (m ³ s ⁻¹) / speed U (m/s) of the water flow	Distance <i>x</i> between the instant discharge and the site of interest (km)	Maximum concentration <i>C_{max}</i> measured "on site" (ppb) / travel time (hours:minutes)	Maximum concentration C_{max} calculated by the warning system (ppb) / travel time (hours:minutes)
SOARES et al., (2010) / Campaign 1 - section P. Policial	0.5 / 12.0	18.45 / 0.55	20.0	6.3 / 10:10	6.3 / 10:05
SOARES et al., (2010) / Campaign 2 - section P. Policial	0.5 / 14.0	32.42 / 0.64	20.0	4.3 / 08:50	4.2 / 08:40
RIBEIRO (2007) / Experiment 28/05/2006 - section Astolfo Dutra	1.57 / 18.0	38.80 / 0.45	6.0	10.5 / 03:35	10.5 / 03:41
RIBEIRO (2007) / Experiment 06/06/2006 - section Dona Euzébia	1.60 / 27.0	44.30 / 0.40	13.0	4.3 / 08:50	4.4 / 09:00
RIBEIRO (2007) / Experiment 06/06/2006 - section Cataguases	1.60 / 35.0	60.0 / 0.37	36.0	1.4 / 26:40	1.5 / 26:55

TABLE 2. Data used for comparison of system performance against experimental results from literature.

From the results presented in Table 2, it can be seen that the performance of the warning system is very satisfactory when comparing to the results measured experimentally and calculated with the system.

Figures 10 (a) and (b) show, respectively, input and warning system data for simulated results for the discharge conditions presented in Table 2, considering the experiment reported by SOARES et al. (2010), Campaign 1 - section P. Policial.

It is noteworthy that there are virtually no scientific reports addressing modeling the soluble pollutants dispersion in rivers of medium size, with flow rates between 10 m^3 /s and 100 m^3 /s, using tracer techniques and analytical equations of one-dimensional transport of conservative soluble pollutants. The Hydrus system (GUEDES et al. 2007), however stands out, that was developed to analyze the dispersion of conservative soluble pollutants, and uses the convolution technique to estimate the impact of continuous discharge in a downstream section.



FIGURE 10. (a) Input data to simulate the effect of a continuous discharge of effluent in a section located 20.0 km downstream; and (b) Effect of instantaneous discharge of a soluble substance in a section distant 20.0 km from the discharge.

A difference between our system and Hydrus, is that the system developed in this work, called "Dispersion", also allows estimating the environmental impact by convolution techniques, of continuous discharge, with the possibility of simulations of instant discharge and to obtain the coefficient of dispersion from experimental results or empirical equations coupled to the system. It also allows the generation of a summary report that outlines the main information related to the discharge, allowing rapid decision-making in case of accidents with soluble pollutants (Figure 11).



FIGURE 11. Summary report generated by the system.

CONCLUSIONS

The computer system developed herein allows determining the value of the longitudinal dispersion coefficient (D_L), and from this, to assess the effects of instant or continuous discharges of soluble effluents in a particular downstream section of a water stream.

The comparison made between the experimental results of campaigns carried out "on site" with tracers, with the results generated by the warning system showed an excellent performance in predicting the transport of a soluble pollutant, in the section of interest downstream of the discharge, from information of a few parameters of the flow.

The system allows generating a summary report containing information from the time of arrival and travel of the pollutant cloud in a particular section of interest, contributing significantly to the management of water resources, as it enables to proactively warn users of water from a river basin, especially in situations of accidental discharges of potentially toxic substances.

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