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A mathematical model for the simulation of the Magdalena River in the city of Barrancabermeja, Colombia

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Abstract. The integration of mathematical models allows the simulation of the spatiotemporal behavior of water quality parameters of a river. The representation of reality and different scenarios through simulation makes it possible to know the variations in water quality of a receiving water source associated with liquid discharges. Therefore, for this study, the mathematical model QUAL2K was applied to simulate the water quality of the Magdalena River in the section that crosses the city of Barrancabermeja, Colombia. For this purpose, a database of hydro-climatological records from 1977 to 2020 was used. Among the analyses, dissolved oxygen and biochemical oxygen demand were considered as water quality parameters. As a result of the initial data processing of the distribution tests and Kolmogorov goodness of fit, the best fit with the normal distribution was obtained for the estimation of flow rates. The concentrations of the water quality parameters dissolved oxygen and biochemical oxygen demand were represented in the mathematical model, which shows the dilution capacity of the pollutant loads of the wastewater, due to the high flow of the Magdalena River in the study section.

1. Introduction

Industrial growth and population concentration increase the negative impact on surface water bodies available as recipients of wastewater discharges or as sources of water supply [1]. This negatively affects the quality of water resources, which makes it necessary to implement strategies for sustainable use. For the control and management of water quality, mathematical models are often used to determine the variations in the water quality of the receiving body associated with the liquid discharge [2].

The free QUAL2K model (River and Stream Water Quality Model), one-dimensional forecast, was developed by the U.S. Environmental Protection Agency (EPA). This software models water quality rivers under steady flow and Windows environment [3]. The simulation model adjusts using as a mathematical tool an algorithm process for calibration [4].

The authors Bui, *et al.* (2019) applied the Qual2k model on the Cau River (Vietnam), in a data scarce sub-basin. The study considered variables such as biochemical oxygen demand (BOD), total phosphorus (TP), total nitrogen (TN) and dissolved oxygen (DO). The model showed that the concentrations of these variables increase downstream of the influent due to the discharge of untreated wastewater from the city [5]. The QUAL2K tool has also been applied in upper Egypt drainage in the Ramganga River, which simulated parameters of interest to aquatic life such as BOD and DO. In this study, no significant impacts on the parameters were observed [6].

The application of models uses mathematical formulas to make a similar representation of the physical reality of a system, such as a river in this case. Modeling allows the evaluation of the relative benefit through the elimination of different pollutants, and the study of the behavior of surface water sources exposed to discharges of liquid effluents [7]. Water quality is defined by the physical, chemical, and biological attributes that influence the availability of water for human consumption and the different uses to which it is subjected [8].

The objective of the present study is the application of the mathematical model QUAL2K to simulate the water quality of the Magdalena River in the section that crosses the city of Barrancabermeja, Colombia. The simulation of water quality allows knowing the impact generated by the pollutant loads of the liquid waste discharges of the city.

2. Methodology

2.1. Study area

The city of Barrancabermeja is in the province of Mares, to the west of the department of Santander on the eastern bank of the Magdalena River, it has a surface of 1274 km^2, Colombia. The population projection according to the "Departamento Administrativo Nacional de Estadística (DANE)", Colombia, for the year 2020 is 179139 inhabitants. The site determined for the research is the wastewater treatment plant (WWTP) San Silvestre, located in a 7.9-hectare plot of land in Barrio Colinas of the city of Barrancabermeja, Colombia; with coordinates 1,275,000N and 1,275,200N and 1,225,800E and 1,226,200E, 7 km from the discharge of the Magdalena River (Figure 1) [9].

The wastewater from the discharge point is at an average temperature of 25.3 °C, with physicochemical characteristics such as BOD$_5$ ranging between 197 mg/L and 41 mg/L with an average of 109 mg/L, chemical oxygen demand (COD) ranging between 344.5 mg/L and 55 mg/L with an average of 211 mg/L, total suspended solids (TSS) ranging between 235 mg/L and 15 mg/L, and DO average 5.10 mg/L. The current state of the land at the WWTP is covered by stubble-type vegetation, with elevations ranging from 90 - 85 meters above sea level. Precipitation in the area has two alternating rainy and two summer periods, which means that the average annual precipitation is 2992.2 mm [10]. It is proposed that the construction of the WWTP will minimize the negative impact of wastewater discharge, which has a high content of organic load and highly toxic pollutants.
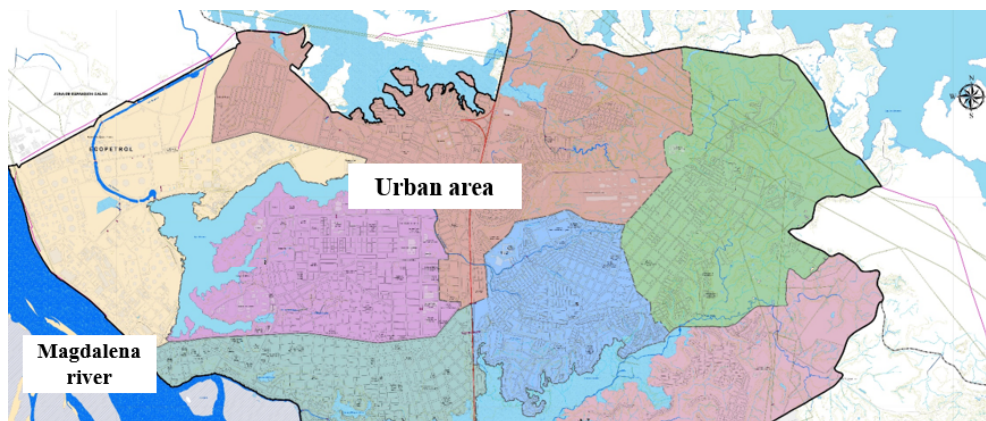

Figure 1. Study area, Magdalena River, Barrancabermeja, Colombia [9].

2.2. Collected information

Flow data were collected from the monthly and daily climatological records established by IDEAM, Colombia, between 1977 and 2020 from the stations located on the Magdalena River, mainly the Galán (23157070) and Barrancabermeja-AU (23157030) stations, which are of the limnigraphic type (LG) located in the city of Barrancabermeja, Colombia. Wastewater quality parameters BOD$_5$ and DO were measured at the discharge point by ILAM between December 2015 - January 2016.

2.3. Data analysis
Based on the monthly flow data, the minimum and maximum flows at the 25, 50, and 100-year return periods were estimated using the Normal, Pearson, Log-Normal, and Log Pearson distribution functions, and the Kolmogorov goodness-of-fit test was applied. The best distribution was selected; in addition, with the daily flows, the monthly average daily flow of the annual series was obtained by taking the values between the first and third quartile expressed in the box and whiskers diagram.

The hydraulic characteristics of the Magdalena River (Manning's roughness coefficient = 0.018; river width = 550 m; river slope = 0.07%, defined by "Aguas de Barrancabermeja S.A. E.S.P"). Based on the minimum, average and maximum flows and the Streeter and Phelps model included in the Qual2k software, the dispersion of BOD_5 and DO downstream of the discharge point was determined and the scenarios of actual discharge and 80% removal estimated for the BOD_5 parameter with the construction of the WWTP were evaluated. The model values were compared with the limit values established in the Technical Regulations of the Drinking Water and Basic Sanitation Sector (RAS) to classify the river as a source of supply [11].

2.4. Mathematical modeling of water quality
The basic equation of the Qual2K model is the advection-dispersion material transport and one-dimensional reaction equations. It solves equations for simulation through a finite difference scheme [3]; Equation (1) shows the general balance for a concentration of the Ci component in the range of i [2].

$$\frac{dc_i}{d_t} = \frac{Q_{i-1}}{V_i}\, c_{i-1} - \frac{Q_i}{V_i} C_i - \frac{Q_{out,i}}{V_i} C_i + \frac{E'_{i-1}}{V_i}(c_{i-1} - c_i) + \frac{E'_i}{V_i}(c_{i+1} - c_i) + \frac{W_i}{V_i} + S_i, \qquad (1)$$

where Q_i, c_i, V_i, E_i, and W_i are the water quality component concentrations, flux, volume, dispersion coefficient, and external component loading of the i range, respectively. S_i represents the sinks and sources of the constituent. Q is the flux in the range i [2].

3. Results

3.1. Estimation of minimum, mean and maximum flow rates
According to the result of the Kolmogorov goodness of fit test, the normal distribution is the best fit for the estimation of minimum and maximum flows at return periods of 25, 50, and 100 years. Table 1 shows that the maximum flows range between 7355.9 m^3/s and 7936.1 m^3/s and the minimum between 643.3 m^3/s and 407.7 m^3/s respectively.

Table 1. Minimum and maximum flows for the return periods of 25, 50, and 100 years.

RP (Years)	Min. flow (m^3/s)	Max. flow (m^3/s)
25	643.3	7355.9
50	519.2	7661.3
100	407.7	7936.1

Note. RP = Return period, Min. Flow = Minimum flow, and Max. Flow = Maximum flow.

Figure 2 shows the box - and - whisker diagram for the monthly daily flows, which shows a bimodal distribution between May - October with the highest flows of 3767.2 m^3/s and 3745.8 m^3/s, February - August with the lowest flows of 1922.7 m^3/s and 2040.7 m^3/s, respectively. Regarding water discharge, we worked with the maximum instantaneous flow for the year 2038, estimated at 2.56 m^3/s.
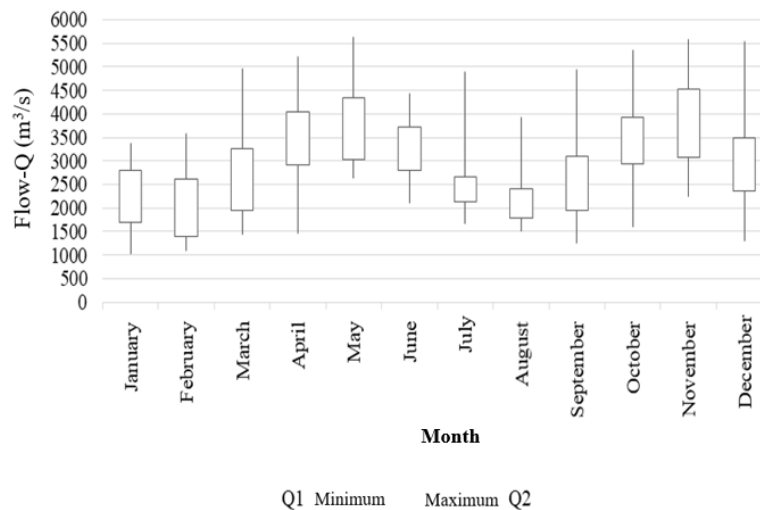
Figure 2. Box-and-whisker plot of monthly mean daily flow rates.

3.2. Model application

As a result of the dispersion of the BOD_5 and DO parameters for the minimum and maximum flow conditions for the return periods of 25, 50, and 100 years, the Spatiotemporal graphs presented in Table 2 were generated.

   Table 2 shows that the BOD_5 at the discharge point for the minimum flows reaches values similar to those recorded at the source before discharge (27.8 mg/L) but begins to decrease over a distance of 6 km because the source flow is 159.2 times greater than the discharge, which is why the Magdalena River tends to purify itself at the same discharge point. Likewise, there is an increase in the DO downstream of the discharge point from 5.10 mg/L to 7.66 mg/L over 6 km.

Table 2. Spatial-temporal dispersion of BOD_5 and DO parameters for minimum and maximum flows.

Distance (Km)	RP (25) Min.*	RP (25) Max.**	RP (50) Min.	RP (50) Max.	RP (100) Min.	RP (100) Max.
			BOD_5 (mg/L)			
0.0	28.12	27.83	28.20	27.83	28.30	27.83
7.5	28.12	27.83	28.20	27.83	28.30	27.83
15.0	27.80	27.80	27.80	27.80	27.80	27.80
			DO (mg/L)			
0.0	7.62	6.59	7.66	6.56	7.69	6.53
7.5	7.62	6.59	7.66	6.56	7.69	6.53
15.0	5.10	5.10	5.10	5.10	5.10	5.10

Note. * RP (25) Min. = Concentration for a return period of 25 years and minimum flow rate.
** RP (25) Max. = Concentration for a return period of 25 years and maximum flow rate.

   The quality parameters BOD_5 and DO, used as indicators for the presence of organic matter in the water body and as a parameter to evaluate the environmental contamination of the area, showed that the bay tends to be purified because the water flow in the bay is greater than the discharge [10].

   Additionally, for the maximum flows the discharge becomes more insignificant compared to the flow of the Magdalena River, the latter being 3100 times greater, which is expected to have greater oxygenation and dispersion of the BOD_5 so that the water source is not affected since the value of the parameter recorded at the discharge point remains constant.

   The simulation of different scenarios was carried out with the construction of a WWTP to comply with the removals established by the Colombian regulations (80% of BOD_5). Table 3 shows the distribution graph of the concentration of wastewater discharge from the WWTP in the river.

Table 3. BOD5 dispersion with 80% removal at the WWTP, for minimum and maximum flows.

Distance (Km)	RP (25) Min. [*]	RP (25) Max. [**]	RP (50) Min.	RP (50) Max.	RP (100) Min.	RP (100) Max.
0.0	27.78	27.78	27.77	27.80	27.76	27.80
7.5	27.78	27.78	27.77	27.80	27.76	27.80
15.0	27.78	27.78	27.80	27.80	27.80	27.80

Note. [*] RP (25) Min. = Concentration for a return period of 25 years and minimum flow rate.
[**] RP (25) Max. = Concentration for a return period of 25 years and maximum flow rate.

According to the provisions of the RAS [11], which establish that the WWTP must remove at least 80% of the pollutant load, the water source has a better dispersion of BOD_5 (see Table 3). The dispersion of the parameters is instantaneous until reaching the initial characteristics of the source (27.8 mg O_2/L BOD_5 concentration).

Figure 3 shows a comparison of the spatiotemporal dispersion of BOD_5 in the simulation scenario with 80% removal and without the presence of the WWTP. The concentrations of the BOD_5 and DO parameters in the 0% and 80% removal scenarios allow classifying the Magdalena River as a source of acceptable quality for supply according to the classification of the RAS, guaranteeing the preservation of flora and fauna (BOD_5 < 50 mgO_2/L and DO > 4 mg/L) [11]. This emphasizes the fact that models allow the representation of physical systems for water resource management [5,12].
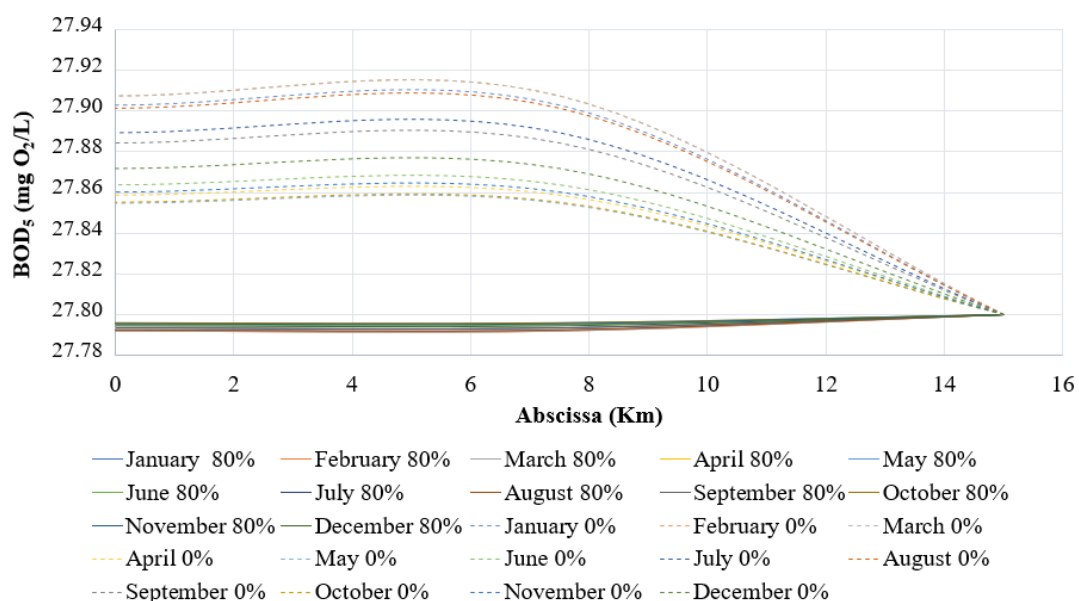

Figure 3. BOD_5 dispersion with 80% removal at the WWTP and without removal, for daily average flows.

4. Conclusions

This research made it possible to use mathematical modelling as a tool to represent the quality of the Magdalena River in the section that passes through the city of Barrancabermeja, in terms of BOD_5 and DO parameters. The simulation with QUAL2K made it possible to represent the physical system of the degradation kinetics of the modelled parameters (BOD_5 and DO) using mathematical formulas. This, mathematical model was able to simulate the dispersion of water quality parameters, showing that at present the Magdalena River in the study section tends to be purified at the same discharge point. The Magdalena River for the flows it carries is capable of instantly reaching the initial characteristics of the source without any removal treatment so that for the most unfavorable condition presented in the 100-year return period at the minimum flow, the source is not affected by the discharge.

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