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Use of network theory to model water quality parameters in a hydrological network

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Abstract. In this work we model and simulate water quality parameters in a hydrological network by using a methodology based on network theory and differential equations. We build the Quindío river hydrological network based on network theory using the Gephi software, the maps from "Instituto Geográfico de Colombia Agustin Codazzi" and data reported from "Coorporacion Autónoma Regional del Quindío". Then, we modelled three water quality parameters using differential equations at each node of the network, these are total coliforms, biochemical oxygen demand, and dissolved oxygen. As a result of the simulations, we found high levels of pollution in the area where there is a presence of human settlements and the local industry. Finally, results also showed a possible relationship between the three parameters studied, mainly due to the high concentrations in the same area of the basin.

1. Introduction

Physical, chemical, and biological parameters are used to assess water quality in river basins [1-4]. In general, these parameters, such as faecal and total coliforms, biochemical oxygen demand, dissolved oxygen, among others, are modelled using ordinary or partial differential equations, [5,6]. However, these models lack showing a general perspective because they assume the river as a unique channel and do not take in to account possible multiple branches and interactions with water streams that shape a hydrological network as a whole. Alternatively, with the theory of networks, we can describe a global panorama of the degree of contamination of the river basin. Furthermore, with the theory of networks, it is possible to infer which places in the network are susceptible to new sources of contamination [7-10].

Therefore, the objective of this work is to present a model of water quality parameters in a hydrological network with an application in the study of total coliforms, biochemical oxygen demand, and dissolved oxygen on the Quindío river basin in Colombia. To accomplish this goal, we use a methodology that combines network theory and differential equations to create the computational model.

2. A mathematical model based on network theory

We based the methodology on the work done by the researchers Wu, *et al*. [7]. We start by the network construction. Then we build the hydrological network of the Quindío river based on geographic information. Finally, we study the dynamics of some water quality parameters on the network.

2.1. Network construction

We classify the nodes of the network according to some characteristics such as [9-11]:

- Natural nodes: are nodes that have no human intervention. They usually represent the headwaters of rivers or streams.
- Artificial nodes: in these nodes there is intervention or human control, for example, monitoring stations, sewage and, non-wastewater discharges, water transfer projects, among others.

According to Wu, *et al*. [7], the edges represent the connection channel or the junction of rivers or streams. Then we classify the edges into:

- Serial connection: is a sequence of edges that are joined by a node.
- Parallel connection: are those edges that share two nodes.
- Mixed connection: occurs by joining the serial and parallel connection.

2.2. Hydrological network of the Quindío river

We used the following information to build the hydrographic network of the Quindío river basin: the software Gephi, Python coding, the maps of the “Instituto Geográfico de Colombia Agustin Codazzi”, and the reports of “Coorporacion Autónoma Regional del Quindío”. Figure 1 shows the graph of the hydrographic network of the Quindío river.

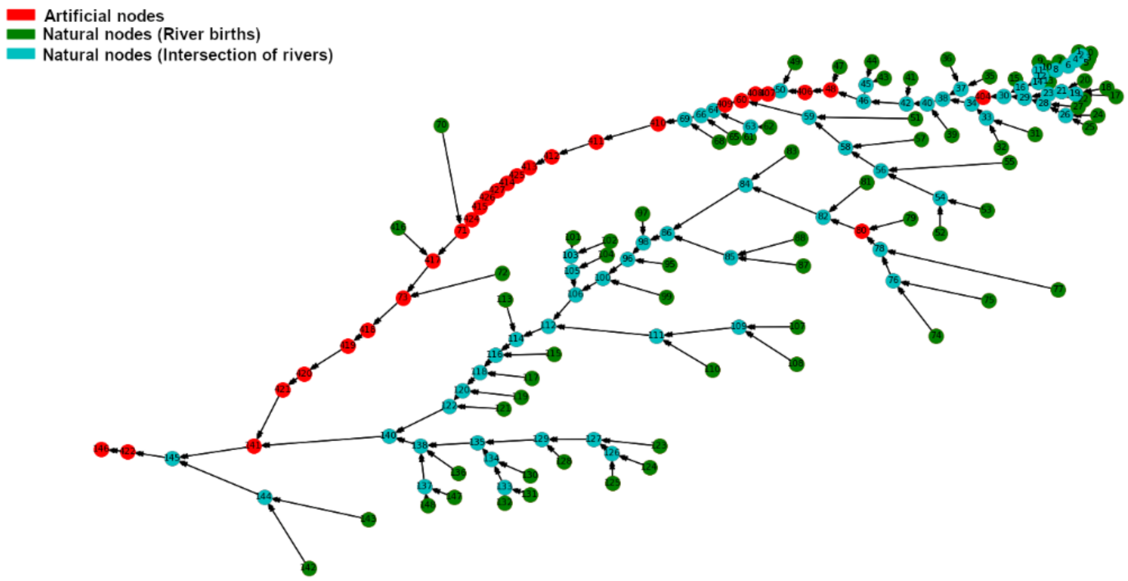

Figure 1. Representation of the Quindío river hydrographic network.

The network in Figure 1 represents a directed graph or digraph [11]. It has 163 nodes, the green and light blue nodes are natural nodes, the green nodes are the head of stream rivers, and the light blue nodes are the intersection of rivers or streams. The red nodes are artificial. Similarly, the network has 163 edges of different types of connections (serial, parallel, and mixed).

3. Dynamics of some water quality parameters

In this section, we present the model of three parameters with the theory of networks and differential equations. These are total coliforms (TC), biochemical oxygen demand (BOD) and dissolved oxygen (DO).

3.1. Total coliforms

To model the total coliforms, we used a decay model [12]. As shown in Equation (1).

$$\begin{cases} \frac{dC}{dt} & = & -kC \\ C_0 & = & c(0) \end{cases} \tag{1}$$

The solution to the initial value problem in Equation (1) is a negative exponential function, which primarily reflects the behavior of coliforms, where C is the concentration of coliforms, t time and k is the decay rate as shown in Equation (2). To run simulations, we consider parameter k, degrading coliforms by 90%.

$$C(t) = C_0 e^{-kt} \tag{2}$$

3.2. Biochemical oxygen demand and dissolved oxygen

For this research we used the system proposed in Equation (3).

$$\begin{cases} \frac{\partial L}{\partial t} = -v\frac{\partial L}{\partial x} - K_r L \\ \frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} - K_d L + K_a C_s - K_a C \end{cases} \tag{3}$$

With v: average flow rate, L: total amount of organic matter remaining in t (t being time), K_r: total BOD removal rate, C: resulting concentration of DO in water, K_d: deoxygenation constant (1/day), L: total amount of organic matter remaining in t, K_a: coefficient of reaireation, C_s: saturation oxygen.

The solution of the system of Equation (3), was obtained from the method of the characteristics of partial differential equations (PDE), where the initial values for the simulation of each scenario, were taken from the different reports and data provided by “Coorporacion Autónoma Regional del Quindío” and “Empresas Públicas de Armenia”. In the event that some river or stream will not have DO and BOD information, a standard value was taken for each of these quality parameters, obtained from the literature; these values are 7.5 mgO_2 for DO and 4 mgO_2 for BOD. The solution of the system in the Equation (3) is shown in Equation (4).

$$\left. \begin{array}{c} L(x,t) = \alpha e^{-K_r t} \\ C(x,t) = \frac{\alpha K_d}{K_a - K_r} e^{-K_r t} + C_s + e^{-K_a t}\left(\beta + \frac{\alpha K_d}{K_a - K_r} - C_s\right) \end{array} \right\} \tag{4}$$

4. Simulations and results

For the total coliforms, we simulate with 200 iterations. The simulation showed that the max concentration occurs in the lower middle zone of the basin, where there is the presence of industrial zones. We observe in Figure 2 that the nodes with higher concentration are those appearing in light green, and those in yellow, show the highest concentration, with levels of up to 10^8 most probable number (MPN).

Similarly, nodes with a lower presence of coliforms appear in dark tones. The final node of the basin has levels of 10^4 MPN, showing relatively high concentration, which tell us that at that point, the river water is not suitable for human consumption. This is alarming, because the Quindío river flows into the La Vieja river, and from the latter, municipalities in the department of Valle del Cauca in Colombia take this water for supply.

Regarding the physical-chemical parameters, BOD and DO, along with the hydrographic network of the Quindío river basin, considering its 72 km length, Figure 3(a) shows the behavior of BOD in the network (after 200 iterations), where the color scale shows how the greater the BOD contribution over the basin is, the values are close to 10^4 (yellow color), while the lower BOD contribution values will approach 0 (red color). On the other hand, in Figure 3(b), we observe how the behavior of the DO in the basin is (at 200 iterations), where the color scale shows that the higher the DO in the basin, the values approximate at 10^2 (yellow color), on the contrary to lower DO in the basin the values will approximate 6×10^0 (red color).

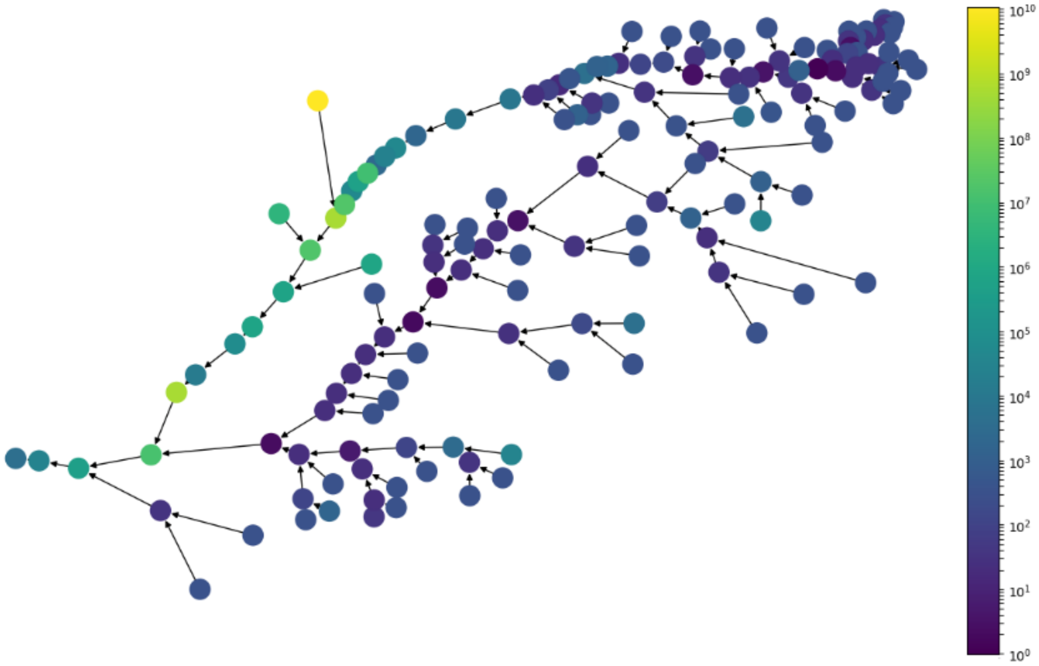

Figure 2. Total coliform concentration in the Quindío river hydrographic network.

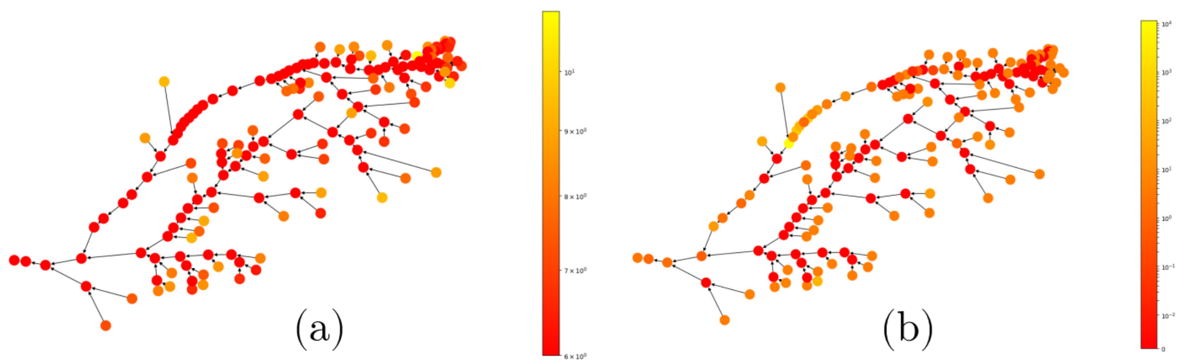

Figure 3. BOD and DO concentration in the Quindío river hydrographic network.

5. Conclusions

The representation of the hydrographic network of the Quindío river basin using network theory, allowed to determine which places are prone to relatively high levels of pollution. Also, it shows other areas of the network that are potentially vulnerable, in Figure 2 and Figure 3 we can see the areas where pollution has impacted in the basin. From this work, we can conclude that network theory is an alternative tool to model water quality parameters.

The problem of initial value that was used to model the coliforms, shows that in the lower middle part of the basin is where this factor is most concentrated. The DO was sufficient to show how the coliform population degrades and the high values of these in some areas of the basin, despite having a degradation factor of 90%.

Regarding the BOD and DO, the model showed how these parameters have an impact in the same area as the coliforms. From these, we can infer that these three parameters may be related, but it is something that we can study in the future. Additionally, the model shows agreement with the levels of DO and BOD present in young rivers and at the heads of the stream waters.

Acknowledgments

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