

A Systematic Methodology for Determining Water Quality Objectives through Mathematical Modeling

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Abstract

As a first step towards the restoration of the Ranchería River (La Guajira-Colombia), we have set Water Quality Objectives (WQO) with a systematic methodology. This methodology consists of initially establishing desirable WQO, consistent with current and potential uses; then it is checked whether the current quality status meets them; afterwards, a feasible sanitation plan is defined for the medium-term (acting on point-wise loads) and for the long-term (on diffuse loads) trying to attain the chosen OCA. Through water quality simulation model (QUAL2KW in our case), suitably calibrated, the corresponding level of achievement of such desirable OCA is hence assessed. Typically, it is necessary to reduce the expectations (WQO targets), especially in the long-term because they can only be achieved with challenging interventions on diffuse sources. The newly determined targets are hence the operational ones. However, also the desirable OCA are useful as a stimulus for start a long-term process. The proposed methodology is useful for any Water Resource Management Plans (WRMP) in Colombia and also in other countries as it avoids the usual error of setting non-attainable WQO that leads to frustration and sometimes to escaping to comply with environmental responsibilities.

Keywords: water quality objectives (WQO), mathematical modeling, QUAL2KW, diffuse sources, river

1 Introduction

The rivers contamination is a very worrying issue worldwide. The countries make efforts to achieve a comprehensive management of water resources. In this sense, legislation defining work routes is issued; worth of mention are: EU with Directive 2000/60/CE [1] and USA with the Clean Water Act since 1972 [2]. Colombia, since 2010, has implemented a system of water resources management, which is based on the Water Resource Management Plans (WRMP). WRMP requires the establishment of Water Quality Objectives (WQO). These are defined as the set of thresholds (targets) of water quality variables that are used to define the suitability of the water resource for each given use. WQO in other countries are known as environmental objectives, Sweden defined them as a distinctive feature of their environmental policy in the early 2000s [3]. The EU defined its environmental objectives with Directive 2000/60/EC.

A serious problem exists when it comes to establishing WQO for a water body: experience shows that in most cases the objectives remain as desires and reality is not achieved. The Colombian norms [4] do not escape this reality and in effect they require the definition of WQO in the short (2 years), medium (5 years) and long-term (10 years), but do not require a priori verification of their ability to reach them. Actively complying with the WQO implies sufficient technical, socio-economic and cultural ability, as well as a strong political will that often, at a (WQO) level, is not capable of facing strong economic interests.

To comply with the WQO, it is necessary to reduce the pollutant loads that the water bodies receive, information that in the great majority of cases is not available in detail [5]. Despite several decades of research and financial commitment, Colombia still has deep weaknesses and inefficiencies in the treatment of point sources: only 48.21% of municipalities treat wastewater (<https://goo.gl/fJ2uvi>). But diffuse (non-point) pollution remains a major problem that threatens the health of ecosystems worldwide [6]. Diffuse pollution is a complex problem with several causal factors, with multiple pathways surrounded by uncertainty and ambiguity [7]. In Colombia, the WQO for several rivers have been established [8], some of them present aspects similar to the one discussed in this paper, with differences in the consideration of diffuse loads, which is the most complex and contributory source of pollution in many rivers of the world [6, 7, 9, 10]. Such experiences do not present a systematic methodology to set the WQO. Defining achievable quality objectives by verifying a priori their feasibility allows planning and implementation of interventions in a more effective and efficient way, preventing the investment from being fruitless. It is

with this criterion and focus that the WQO for the Ranchería River, the main source of the department of La Guajira, Colombia, were set up in the research described in this article.

2 Methodology

2.1 Area of study

The study was carried out in the Ranchería river (figure 1), the main water body of the department of La Guajira- Colombia. The water quality assessment and the necessary monitoring were carried out from downstream of the El Cercado dam (N: 10° 54'29.31", E: 73° 00'38.84"), down to its mouth in the Caribbean Sea (N: 11° 33'16.1", E: 72° 54'10.5") corresponding to a length of about 235 km (total length of the river is 284 km), of which we modeled 225 km due to the mixing of seawater at the mouth.

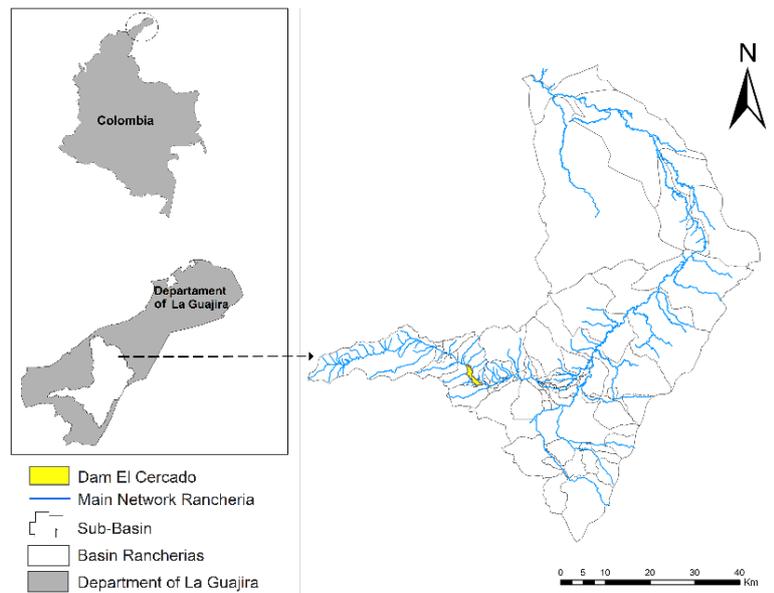


Figure 1. Location of area and basin under study

2.2 Conceptualization of the methodology used

Initially, desirable WQO (more precisely the associated quality thresholds) were established according to the criteria or standards established by Colombian regulations based on current and potential uses of the river; then, we followed a methodological scheme (figure 2) that systematically describes the process developed to set the reachable WQO.

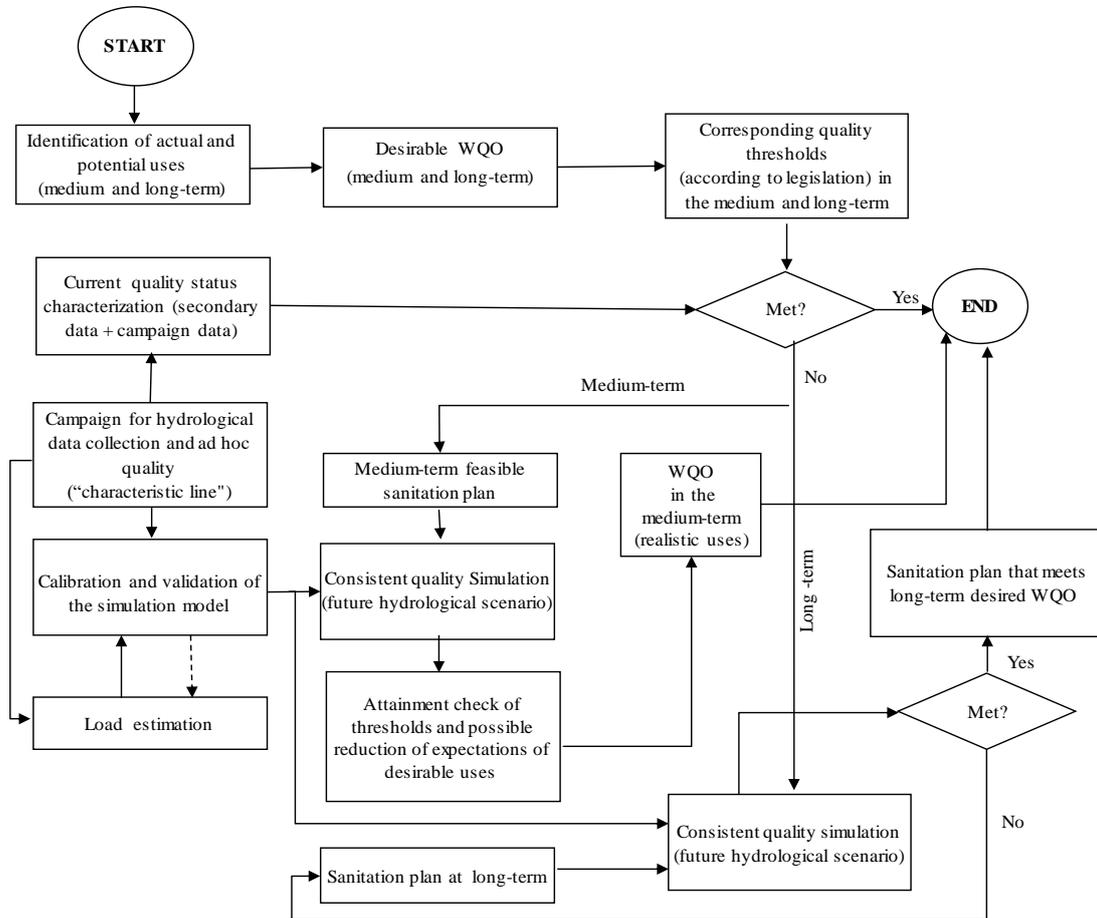


Figure 2. Methodological flow diagram to establish the water quality objectives of the Ranchería river

2.2.1 Current and potential uses. The field trips, the application of surveys to users and the secondary information allowed knowing the current uses; with this information, the maps of land use and information related to the productive systems, the potential uses were defined. The river was divided into 7 homogeneous reach by use.

2.2.2 Water quality thresholds. According to current and potential uses, the quality thresholds required by the Colombian standard were considered [11]. When several uses were presented in a reach, the most demanding requirement was taken.

2.2.3 Desirable quality objectives. The Corpoguajira Regional Environmental Authority had established the WQO of the Ranchería River for the period 2004-2016. We assume this WQO as short term (2 years). Therefore, in this investigation it was decided to determine the desirable WQO in the medium and long-term.

2.2.4 Sampling campaigns for model calibration. First, a preliminary campaign was carried out to establish the quality and quantity measurement techniques, choose the exact sites for the samplings and to determine the transfer time of water from one station to another. Then a specific campaign was designed and conducted to collect data useful to calibrate the simulation model of water quality (QUAL2KW). This campaign was organized in the dry season assuming a plug-flow system that ignores the dispersion and assumes a Lagrangian point of view [12], this assumption was supported by the "Extended Dobbins" criterion [13]. In the dry season, Rancheria River usually presents its worst quality conditions [14]. Through this campaign also the water balance of the river was set up. To ensure the presence of steady-state conditions, agreements were made so that during the campaign no maneuvers were carried out at the El Cercado dam that could alter the flow. Measurements were also made to determine the "state" of quality in 27 sampling stations in the main river stem and samples were also taken in all its relevant tributaries and discharges to determine loads. The quality variables were measured in the Environmental Quality laboratory of Universidad del Magdalena (Colombia) following the procedures established in the Standard Method [15].

2.2.5 Characterization of the quality status. With the historical water quality and campaign data, compliance with the requirements requested by Colombian regulations was verified for each current and potential use. To this aim, water quality indices (ICA) were computed and analyzed [16].

2.2.6. Point and diffuse pollutant load. Point loads (tributaries and discharges) were obtained directly from the campaigns (i.e. flow times concentration). The industrial loads were estimated based on the average values of the historical measurements reports sent by Carbones del Cerrejón Limited (hereinafter Cerrejón) to the Regional Environmental Corporation (Corpoguajira). For the diffuse loads (agricultural and livestock) first a gross estimation of potential diffuse loads was conducted based on literature coefficient and knowledge of local land use and magnitude of cattle; then, during the calibration of the QUAL2KW model a reduction coefficient was determined to obtain the effective loads that reaches the river. Finally, ad hoc corrections were made based on what the measurements reflected. We stress that the correct process is to estimate the quality of the river (state) from the known loads (cause) and not vice versa; but there was no other option to arrive at a coherent data set. To this aim export coefficients for each pollutant should be available, but this information is still a global challenge [5, 9, 10, 17].

2.2.7 Calibration and validation of the simulation model. With the final campaign data, the model was calibrated (QUAL2KW version 5.1) in three stages: i) an initial qualitative adjustment criterion (visual), ii) refinement with automatic optimization, iii) manual adjustment to the variables of interest.

Since some variables of the model do not coincide with the "parameters", that is the variables required by the Colombian norm for the different uses, it was necessary to establish some correspondence rules as follows:

i) chlorides (Cl^-), sulfate (SO_4^{2-}), total coliforms (TC), oils and grease (O&G) are not considered by the model, but they are by the norm; therefore, in order to check compliance of current status and simulated plans qualitative considerations, based on historical data and measurements obtained in the campaign, were adopted;

ii) The TCs, not considered by the model, were determined from the campaign data using the relationship $\text{FC}/\text{TC} = 0.74$;

iii) The biochemical oxygen demand (BOD) and total suspended solids (TSS) are not required in the Colombian standard, but are considered by the model and obviously are important variables to determine water quality; for BOD it is considered that a clean river must have a BOD value <3 mg/L [18]; to establish the value of the SST, the historical values measured in the low season were adopted;

iv), the model considers the concentration of nitrate (NO_3^-), as the sum of nitrite (NO_2^-) and nitrate (NO_3^-), because the first transforms very quickly into the second [19]; therefore, the values measured in the campaign for these two forms of nitrogen were added as input to the model.

2.2.8 Medium-term feasible sanitation plan. For the desirable WQO for the medium-term, compliance with the regulatory requirements of current uses was considered. In this sense, the water quality found in the historical and campaign measurements were not satisfactory; therefore, we defined a feasible sanitation plan in the medium-term (% reduction of point-wise loads) that would best move towards the achievement of the desirable WQO. This allowed enlightening the role of domestic and industrial loads (Cerrejón).

2.2.9 Simulation of future low-end quality and setting of achievable medium-term objectives. The river was divided into 26 reaches considering hydrology and geomorphological aspects. The hydrology of future, hypothetical conditions adopted as scenarios, was obtained via simulation using the WEAP model (www.weap21.org) and its outputs were inserted (input) into the QUAL2KW. With the calibrated model, the feasible sanitation plan was simulated in the medium-term. The quality obtained was compared with the desirable medium-term objectives, verifying which uses remained acceptable and choosing less demanding uses where the check was negative; these final uses were established as achievable objectives (WQO in the medium-term).

2.2.10 Necessary rehabilitation to achieve long-term WQO. The combination of sanitation options capable of meeting the thresholds of desirable WQO in the long-term was iteratively sought. The diffuse loads linked to livestock were identified as responsible for the breach of quality thresholds; therefore, it was

necessary to intervene on them. In this case, in addition to medium-term sanitation, the reduction of agricultural loads with a reduction factor of $k < 1$ was considered until verifying that the desired thresholds were achieved. The set of loads reductions constitutes hence the long term plan.

3 Results and discussion

With the field survey the current uses in each reach were classified according to the following ones: human and domestic consumption whose drinking water requires conventional treatment (A); human and domestic consumption directly from the source (B); agricultural, irrigation crops other than fruits that are consumed without removing the peel and short-stemmed vegetables (C); recreation through primary contact (D); dilution and assimilation of contaminant (E); preservation of flora and fauna (F); livestock (G) and industrial (H). In the long-term B should no longer exist.

3.1 Thresholds and characterization of water quality status

Table 1 shows the quality requirements according to current and potential uses. The requirements can be absent (A) as in the case of Oils and Grease (O&G), or not required by the norm (N) for a particular use or a minimum-maximum range. (According to the historical data and measured in the campaign, the average temperature in reach 3 was 25 °C and in reach 7 was 28 °C, thus determining the equivalent of 70% oxygen saturation)

3.2 Desirable quality objectives in the medium and long-term

For medium-term desirable WQO, the requirements of the current uses described in table 1 are considered. The long-term desirable WQO that are expected to meet the potential uses are presented in table 2. The most demanding use in terms of coliforms is the recreational with primary contact, which is present in the middle and lower river segments; therefore, the same requirements are set for them. In historical and campaign measurements, oils and grease (O&G) were less than 1 mg/L, except in reach 4 and 5, where 20 mg/L and 35 mg/L were recorded respectively; it is recommended that these variables should be verified and monitored periodically.

In the first two reaches, a concentration of $\text{NO}_2^- \leq 0.1$ was considered (much lower than that required in the standard). The decision was justified because the conventional treatment does not remove nitrifying compounds and also the determined concentrations are lower than 0.1 mg/L, which would prevent compliance with the demands of water for human consumption. Nitrite is rapidly converted to nitrate, which justifies low concentrations [19]. For the same normative requirements indicated above, a desirable concentration of $\text{SO}_4^{2-} \leq 250$ mg/L was established.

Table 1. Quality requirements of the Colombian standard according to each use of the water resource

Reachs	Variables										
	Uso	OD %/(mg/L)	pH Ad	NO ₂ mg/L	NO ₃ mg/L	NH ₄ ⁺ mg/L	Cl ⁻ mg/L	SO ₄ ⁻ mg/L	CT NMP/100 mL	CF NMP/100 mL	O&G mg/L
1	A,C,G	N	5.0-9.0	<10	<10	<1	<250	<400	<20000	<2000	A
2	B, C,F,G	N	5.0-9.0	<10	<10	<1	<250	<400	<20000	<2000	A
3	B,C,D,F,G,H	70/5.7	5.0-9.0	<10	<10	<1	<250	<400	<1000	<200	A
4	B,C,E,F,G	N	5.0-9.0	<10	<10	<1	<250	<400	<20000	<2000	A
5	E,H	N	N	N	N	N	N	N	N	N	N
6	B,C,F,G	N	5.0-9.0	<10	<10	<1	<250	<400	<20000	<2000	A
7	D,E,G	70/5.5	5.0-9.0	<10	<90	N	N	N	<1000	<200	A

Table 2. Desirable long-term quality objectives

Reach	WQO		DBO mg/L	OD mg/L	pH Ad	NO ₂ mg/L	NO ₃ mg/L	NH ₄ ⁺ mg/L	Cl ⁻ mg/L	SO ₄ ⁻ mg/L	CT NMP/100 mL	CF NMP/100 mL	SST mg/L
	Modelo	Qual2kw											
1	1	1	≤3	>6.5	6.8-8.5	<0.1	<10	<1	<25	<250	<1000	<200	<100
2	2	2	≤3	>6	6.8-8.5	<0.1	<10	<1	<25	<250	<1000	<200	<100
3	3.4	3.4	≤3	>6	6.5-9.0	<1	<10	<1	<25	<250	<1000	<200	<150
4	5 a 8	5 a 8	≤3	>6	6.5-9.0	<1.5	<10	<1	<50	<250	<1000	<200	<150
5	9 a 11	9 a 11	≤3	>6	6.5-9.0	<1	<10	<1	<80	<250	<1000	<200	<150
6	12 a 21	12 a 21	≤3	>6	6.5-9.0	<1	<10	<1	<80	<250	<1000	<200	<200
7	22 a 26	22 a 26	≤3	>6	6.5-9.0	<1	<10	<1	<80	<250	<1000	<200	<200

3.3 Calibration and definition of loads (point and diffuse)

It can be say that, in spite of the limitations, the calibration of the model is satisfactory since there were hydrological uncertainties and scarcity of data to determine the contribution of the diffuse loads and given the complexity of the physical and chemical processes involved. To have a systemic view of the loads, they were distributed along the river. The point load (kg/day) was expressed in terms of distributed load (kg/km/d) by dividing by a conventional distance of 100 m. Figure 3 shows the point and diffuse BOD load along the river as an example.

Figure 4 shows the potential BOD loads point (civil) and diffuse (agricultural and livestock) estimated in the Ranchería river basin. It was determined that the main factor in the generation of load is the presence of livestock, which largely generates diffuse loads, much more than agricultural fertilizers contribute, and much higher than the contribution of the civilian population and even of the industrial activity of the Cerrejón. Therefore, the policy of reduction of loads should be focused on the agricultural sector, especially the extensive cattle ranching present in the upper and middle part of the basin. This policy would envisage not only reducing the number of animals per unit area, but also the introduction of appropriate technological to handling excrete.

Despite the foregoing, Colombia still focuses its efforts on the control of point sources that is not the main cause of the pollution of the Ranchería River, as it happens in many parts of the country and of the world.

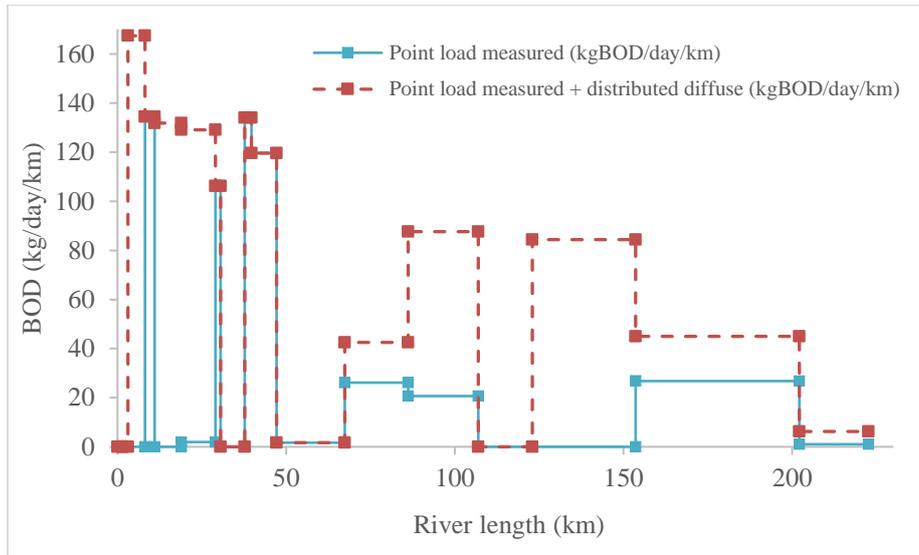


Figure 3. Comparison between the measured and diffuse point loads reconstructed for the BOD

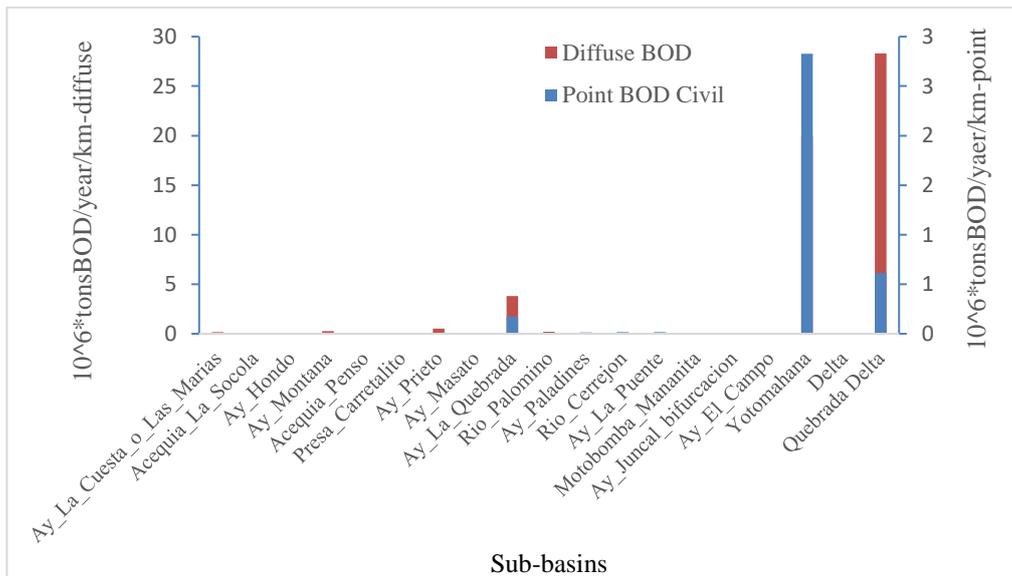


Figure 4. Potential load of domestic and agricultural BOD by sub-basin.

To name some cases, in the Lean-China River they found that diffuse sources are the largest contributors of nitrogen [20] as well as the ChangLe River in China [17]. In the Massachusetts Rivers in USA, a significant decrease in total phosphorus concentration is reported only 15 years after implementing effective management practices for diffuse sources [2]. In Enborne River in England the highest concentrations of phosphorus and nitrogen came from diffuse sources related to rainfall [21]. In the basin of the rivers Ayr and Lunan (UK) the greater contribution of pathogenic organisms like the E. Coli is due mainly to the diffuse sources of cattle [10]. Along the Hardy River-border between Mexico and the USA, they found a high contamination of E. Coli from feces coming from a population of birds that use vegetation as a resting area [22].

There is no recipe to determine the amount of pollutants that diffusely reach the mainstream. The diffuse sources load rises a complex problem that began to face in the late 90s [3]; its estimate, contribution, treatment remains a challenge [1, 7, 10] also because its concentration varies between the period of rain and drought [21].

This discussion shows that Colombia, like many developing countries, must face the challenge of reducing diffuse pollution, which implies great knowledge challenges and, above all, a high financial cost. England spent around £8 million to deal with diffuse pollution in 2008-2009 [23]. In this sense, EUA with the Clean Water Law gives great importance to contamination by diffuse sources [2]. Sweden in the period 1999 - 2011, decided to address this problem [3]. The EU also defined in a coordinated way Directive 2000/60/EC and attach great importance to all forms of water pollution [24]. This regulation and programs up to this level have not occurred in Colombia where it is estimated that only 10% of the systems built have an adequate functioning (<https://bit.ly/2yfdwtY>).

3.4 Medium-term quality objectives according to feasible sanitation plan

In this case, the only plan considered was municipal sanitation. Reduced civilian loads were simulated according to the Plans of Sanitation and Management of Effluents (PSME) or reduction to 80% for the municipalities where PSME did not exist. The results of this simulation are presented in table 3. To verify the effect of Cerrejón loads, the industrial load is eliminated in the simulation; the results showed similarity with those obtained in municipal sanitation. Although a little better, these results were not considered due to the lack of regulatory requirements for Cerrejón to eliminate these loads.

The medium-term desirable objectives are met with the requirements, except "coliforms", which is only met in reach 4 (of the WQO) where we have values close to 1000 NMP/100mL and in reach 5 where it is not required by the industrial use; it is also not met with the requirement of dissolved oxygen in reach 7.

Table 3. Results of the municipal sanitation simulation: reduced civilian loads.

Reach		Distance (km)	BOD (mg/L)	DO (mg/L)	pH (Ad)	NO ₂ +NO ₃ (mg/L)	NH ₄ ⁺ (mg/L)	CF (NMP/100 mL)	SST (mg/L)
WQO	Model								
1	1	4.02	3.43	4.94	7.45	0.110	0.145	3391	18.04
2	2	8.84	3.84	5.97	7.24	0.140	0.141	9572	26.06
3	3	15.40	4.65	7.51	7.58	0.181	0.129	6940	26.68
3	4	23.42	4.56	7.07	7.85	0.160	0.103	3381	21.73
4	5	33.98	3.80	6.12	7.81	0.156	0.077	1073	19.42
4	6	42.17	3.81	6.04	7.94	0.173	0.077	1250	17.26
4	7	55.50	3.37	5.38	7.89	0.269	0.094	1050	16.96
4	8	71.50	2.97	5.55	7.91	0.108	0.082	332	15.33
5	9	87.95	3.68	6.61	8.00	0.147	0.091	2674	17.64
5	10	102.08	5.05	5.39	7.99	0.621	0.281	21947	33.87
5	11	104.66	5.20	5.15	7.98	0.636	0.277	28138	36.19
6	12	110.41	5.64	5.79	7.98	0.701	0.277	25347	41.36
6	13	119.81	4.95	4.08	7.92	0.768	0.256	8334	40.29
6	14	126.49	5.27	3.06	7.87	0.799	0.259	11792	42.74
6	15	136.32	6.67	2.58	7.84	0.814	0.278	25280	50.50
6	16	148.92	8.15	1.90	7.79	0.648	0.274	24184	59.06
6	17	156.83	8.53	1.80	7.78	0.504	0.257	21903	61.08
6	18	165.25	10.93	7.13	8.13	0.069	0.232	6758	47.92
6	19	177.81	9.84	4.60	7.98	0.312	0.174	19971	47.02
6	20	192.89	8.81	3.00	7.89	0.383	0.140	20234	45.63
6	21	204.26	8.01	1.62	7.82	0.511	0.121	24921	44.93
7	22	210.12	7.52	1.05	7.79	0.530	0.112	23385	44.53
7	23	216.33	6.40	1.17	7.77	0.658	0.109	23863	36.90
7	24	221.09	6.01	0.45	7.73	0.676	0.098	21078	36.62
7	25	223.87	5.89	0.44	7.73	0.660	0.095	18523	36.49
7	26	225.10	5.82	0.42	7.73	0.648	0.093	15824	36.41

According to these results, it became necessary to reduce expectations regarding the WQO desirable in the medium-term (table 1), setting the achievable objectives corresponding to the requirements that make possible the following uses: C, E, F, G, H. Although the requirements for human consumption prior to conventional treatment (use A) have not been met, it was identified that in the first reach it is used for that purpose. The above is achieved with a rigorous disinfection to comply with 0.0 coliforms for drinking water (<https://goo.gl/iP32vK>).

3.5 Long-term quality objectives

The simulation of the diffuse loads determined that the civil and industrial loads constitute a smaller fraction of the total loads. The long-term desirable WQO are fully achieved when, in addition to basic sanitation (point loads), a reduction of

diffuse loads is simulated, specifically livestock reduction to 1% and improved Headwater quality with respect to data measured in the campaign as follows: CF decreases from 2820 NMP/100mL to 200 NMP/100 mL; BOD from 3.4 mg/L to 3.0 mg/L and the OD increases from 4.60 mg/L to 7.33 mg/L. To achieve these goals, it is necessary to develop actions that require great efforts. Although it is hard to implement, it is considered sensible because it becomes a stimulus to implement actions to improve water quality.

4 Conclusion

An acceptable calibration of the model was achieved in spite of having data from a single sampling campaign, the diffuse loads issue being the most complex to tackle.

The analysis of point and diffuse loads allowed knowing that the pollution generated by livestock is the major contributor to the deterioration of the water quality of the Ranchería River. It is then necessary for the environmental authority to coordinate strongly with all national and local stakeholders to achieve the joint construction of solutions towards the reduction of the number of animals per unit area and the adoption of appropriate technology for handling excrete.

To achieve the quality objectives achievable in the medium-term, it was necessary to reduce expectations, after the simulation with sanitation measures on civil or domestic (point) loads. Long-term WQO are possible with the reduction of diffuse livestock loads to quite demanding levels, but we have considered it sensible because it becomes a stimulus to implement actions in search of improving water quality. But above all, realistic objectives are defined.

The methodology developed in this research is valid to extrapolate to any river and can be used with any model that correctly simulates water quality, but it is necessary to consider: i) the need to intervene not only on pollutant loads but also on flows, ii) consider times according to the response of ecosystems and the policies of each country, iii) the need for an adaptive approach due to uncertainties and possible evolutions of potential uses; and iv) the verification of obtainable WQO through modeling, often requires reducing expectations.

It is important that each nation defines the interventions, times, and financial support necessary to achieve the WQO; for the case of Colombia very little has been done. The European Union has conducted an interesting exercise on this issue, establishing initial deadlines, very long-term follow-up, continuous updating of the plans, strong economic support and political commitment. In Colombia, WQO are required as an inclusive part of the WRMP, but their verification and compliance is not included in their considerations, which shows a significant institutional weakness.

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