

File S2

B.1. Potable Water Quality

Water quality is a global challenge for potable water distribution systems, especially in smaller systems. The intermittent nature of supply and operation at low speeds can negatively affect water quality throughout the network [1,2]. Traditional methods of measuring physical, chemical and microbiological parameters are not sufficiently effective in evaluating water quality [3]. Therefore, the use of Water Quality Indices (WQI) combined with Geographic Information Systems (GIS) has been widely used to improve water quality assessment [4,5]. Geoprocessing tools, such as Inverse Distance Weighting (IDW), allow for estimation of water quality in areas without direct data and analyzing relationships between water quality and other spatially represented factors [6–8]. By combining WQI with geoprocessing tools, it is possible to improve the accuracy and scope of the assessment of pipeline failure risk and its impact on water quality.

In this context, to evaluate the water quality in each pipeline of the distribution network, four consecutive steps were followed: monitoring planning, potable water analysis, definition and calculation of WQI and use of geographic information systems. These steps allow for the analysis of relationships between water quality and other relevant factors for distribution system management, such as hydraulic parameters (pressure, velocity, and flow), mechanical parameters (length and diameter) and financial parameters (replacement cost of the pipeline). In this way, valuable information was provided for efficient and effective decision making.

B.1.1. Monitoring Plan

Eighty-nine monitoring stations (S1-S89) were defined for the analysis of the variation of the potable water quality parameters in the system, to form a representative sample of the collection points in the network such as: university, schools, hotels, military units, canteens, hospital, commercial establishments (fuel stations, supermarket, banks, barber shop, etc.), residences and lodgings. The distribution of the 89 monitoring stations is represented in Figure B1 and constitutes 10 control areas (A1-A10) in addition to the treatment outlet (A11). At least 12 samples were collected fortnightly for analysis, being 1 (one) for each control area (A1-A10), collected randomly, and 2 (two) immediately after treatment (S89 = A11). The study considered just over three years of monitoring (08/01/2019 to 09/02/2022), with 1040 samples collected during the period, noting that the new sector (crossed by the new pipe presented in Figure B1 connecting S10 to S14) integrated into the system at the end of 2020 was discarded from this sampling due to the unavailability of the data required for analysis.

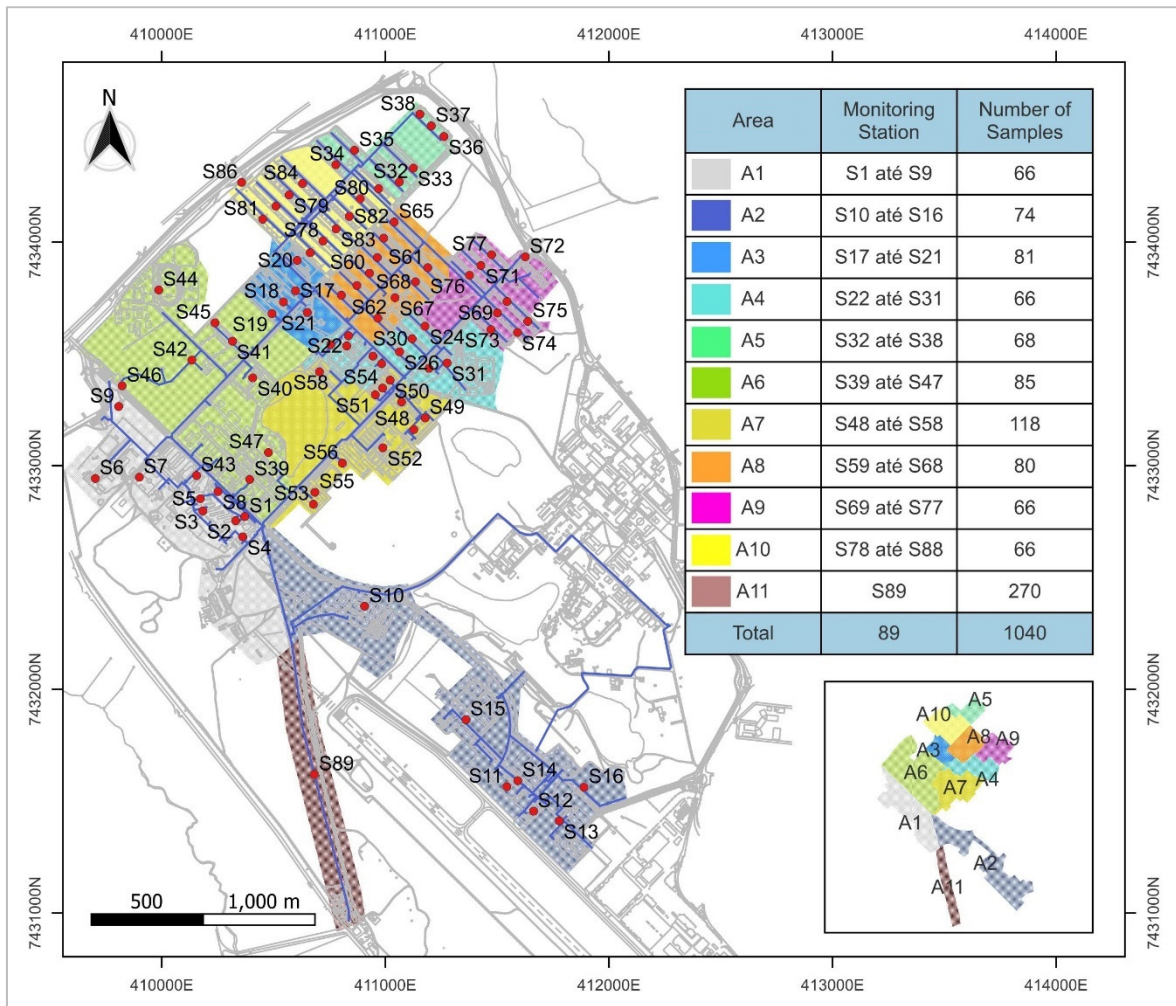


Figure B1. Monitoring Plan

B.1.2. Potable Water Analysis

Sterilized 500ml polyethylene containers were used to collect the samples to the analysis of the physical and chemical parameters. The samples were stored in a thermal container and analyzed in the WTS laboratory. Free residual chlorine (mg/l), apparent color (uH) and total iron (mg/l) were analyzed respectively with the portable colorimeters Pocket II HACH® - Chlorine, Digimed® DM-COR and Pocket II HACH® - Iron. Hydrogen ion potential (pH, dimensionless) was measured by a digital bench pH meter HANNA®, model HI2221, properly calibrated with buffered solutions (pH 4.00 ± 0.02 and 7.00 ± 0.02). The turbidimeter model 2100Q (a portable HACH®) was used to quantify the turbidity (expressed in Nefelometric Turbidity Units, NTU). It was properly calibrated with 0 and 100 NTU solutions.

Sterilized (autoclaved) polypropylene containers (500 ml) were used to collect the samples to determinate the microbiological parameters. These analyses were carried out by the membrane filtration method for quantification of Total Coliforms and Escherichia Coli. This methodology is based on filtering 100 ml of water under negative pressure (vacuum), using a filter membrane with a porosity of $0.45 \mu\text{m}$. The bacteria that presented dimensions larger than the pore of the membrane remained retained on the surface, which was transferred to the Petri plate, containing the selective and differential culture medium m-ColiBlue24®. By the capillarity phenomenon, the medium diffused with the membrane made it possible to contact the bacteria. After 24 hours of incubation at $35 \pm 0.5^\circ\text{C}$, there was the development of Colony Forming Units (CFU) and the count was carried

out for total coliforms (CFU/100ml) when there was growth of red/pink colonies and blue colonies for E. coli (CFU/100ml).

The results of the tests carried out for each physical and chemical and microbiological parameter are available from the corresponding authors upon reasonable request.

B.1.3. Definition and Calculation of the Water Quality Index (WQI)

Among the most widely used methodologies for calculating the Water Quality Index (WQI) are those from the Council of Canadian Ministries of the Environment (CCMEWQI) and the National Sanitation Foundation (NSFWQI) [9,10]. However, due to the flexibility of the parameters considered and the NSFWQI index being particularly sensitive to the standard value used for its calculation, the CCMEWQI with the modifications proposed by Haider [11] was defined for this study, which incorporated the impact of microbial failure in the calculation expression to evaluate water quality, as shown in equation 1.

$$CCME\ WQI_{Mod} = W_1 \times (CCME\ WQI) + W_2 \times (WQI_{MB}) \quad (1)$$

This equation adds the impact of the microbiological parameters (WQI_{MB}) and the application of relative importance weights (W_1 and W_2) to the original index (CCME WQI), a unique weighting scheme (based on the opinion of experts) according to their importance for the different components of a WSS. For water distribution systems, the author [11] proposes equal weights ($W_1 = W_2 = 0.5$), however, different weights were considered ($W_1 = 0.6$ and $W_2 = 0.4$) microbiological parameters already represent high impact in the calculation of the "Water Quality Risk Index for Human Consumption - IRCA" [12]. The IRCA was established in the country of Colombia and has been well received by other countries in Latin America to ensure that the water supplied by the sanitation companies meets the potability characteristics established for human consumption [9,13,14].

For the physical-chemical parameters, the CCME WQI determined by the equation was adopted:

$$CCME\ WQI = 100 - \left(\frac{\sqrt{F_1^2 + F_2^2 + F_3^2}}{1.732} \right) \quad (2)$$

This index is based on the determination of three factors: scope, frequency, and amplitude. Scope (F_1) defines the percentage of variables that have values outside the desired range for the use being evaluated in relation to the total number of considered variables. Frequency (F_2) is found by the ratio of the number of values outside the desired levels to the total number of data from the studied variables [15].

$$F_1 = \frac{\text{Number of failed variables}}{\text{Total number of variables}} \times 100 \quad (3)$$

$$F_2 = \frac{\text{Number of failed tests}}{\text{Total number of tests}} \times 100 \quad (4)$$

The amplitude (F_3) represents the average deviation of the values of the failed test from their respective guidelines. The relative deviation of a failed test relative to the objective is called excursion. Excursions are defined by the following rules. When the test value should not exceed the objective:

$$Excursion_i = \left(\frac{Failed\ test\ value_i}{Objective_j} \right) - 1 \quad (5a)$$

When the test value should not fall below the objective:

$$Excursion_i = \left(\frac{Objective_j}{Failed\ test\ value_i} \right) - 1 \quad (5b)$$

The pH and free residual chlorine (frc: mg/l) were analyzed using both equations (5a and 5b) depending on the defined target range ($6 \leq \text{pH} \leq 9.5$ and $0.2 \leq \text{FRC} \leq 5$). It should be noted that for the free residual chlorine, due to the adjusted measurement range (high 0.1 to 8.0 mg/L) of the Pocket II HACH® - Chlorine colorimeter, values below 0.1mg/L were not detected, so in these cases, the minimum value of the apparatus' low measurement range (0.02mg/L) was considered. For the other physical-chemical parameters, equation (5a) was used.

The collective value by which individual tests are non-compliant is calculated as follows:

$$nse = \frac{\sum_{i=1}^n excursion_i}{\Sigma\ of\ tests} \quad (6)$$

Where *nse* is the normalized sum of the excursions from the objectives.

The F3 factor is then calculated by a formula that scales the *nse* to produce a range between 0 and 100.

$$F_3 = \left(\frac{nse}{0.01\ nse + 0.01} \right) \quad (7)$$

For the microbiological parameters, the WQI_{MB} is as calculated through equation 8.

$$WQI_{MB} = \left[1 - \left(\frac{Total\ number\ of\ failed\ microbiological\ tests}{Total\ number\ of\ microbiological\ tests} \right) \right] \times 100 \quad (8)$$

Table 1 presents the drinking water quality standards according to the requirements of the WHO [16] and Brazil [17] for each parameter. The Brazilian standard is considered for delimiting the acceptable range of "tests" in the presented equations.

Table B1. Drinking water quality standards used in the calculation of CCMEWQI_{Mod}.

Quality parameters	WHO Standard [16]	Brazilian Standard [17]
Residual chlorine (mg/L)	5.0	0.2 – 5.0
Color (uH)	15	15
Iron (mg/L)	*	0.3
pH	8.5	6.0 – 9.5
Turbidity (NTU)	5	5
Total Coliforms (CFU/100mL)	0	0
Escherichia Coli (CFU/100mL)	0	0

* No health-based guideline value is proposed [16]

The calculation of the CCMEWQI_{Mod} was performed for the 89 monitoring stations (S1-S89) considering the results of the tests conducted during the period to assess the water quality in the system. In the calculation of the index, due to the large number of samples, the guidelines of Kilgour [18] were adopted for the exclusion of data associated with extreme events and the results are presented in Table B2

Table B2. CCMEWQI_{Mod} Index Results

Station	CCME WQI									WQIMB			¹ CCME WQI _{mod}	
	failed var.	t.var.	F1	failed test	t.test	F2	Σexc.	nse	F3	Result	failed test	t.test		Result
S1	1	5	20	1	39	2.564	1.000	0.026	2.500	88.27	0	10	100.00	92.96
S2	0	5	0	0	30	0.000	0.000	0.000	0.000	100.00	0	10	100.00	100.00
S3	0	5	0	0	53	0.000	0.000	0.000	0.000	100.00	0	20	100.00	100.00
S4	1	5	20	1	25	4.000	0.007	0.000	0.027	88.22	0	8	100.00	92.93
S5	3	5	60	3	33	9.091	2.240	0.068	6.356	64.77	0	14	100.00	78.86
S6	1	5	20	1	20	5.000	0.533	0.027	2.597	88.00	0	6	100.00	92.80
S7	2	5	40	2	41	4.878	0.087	0.002	0.211	76.73	0	10	100.00	86.04
S8	2	5	40	3	44	6.818	1.493	0.034	3.283	76.50	0	12	100.00	85.90
S9	0	5	0	0	32	0.000	0.000	0.000	0.000	100.00	0	7	100.00	100.00
S10	2	5	40	3	29	10.345	0.633	0.022	2.137	76.11	0	10	100.00	85.67
S11	4	5	80	26	65	40.000	36.608	0.563	36.029	44.33	3	20	85.00	60.60
S12	3	5	60	13	53	24.528	9.180	0.173	14.764	61.62	6	18	66.67	63.64
S13	4	5	80	24	53	45.283	37.575	0.709	41.485	41.77	3	18	83.33	58.40
S14	4	5	80	23	50	46.000	30.724	0.614	38.061	42.37	4	16	75.00	55.42
S15	3	5	60	11	58	18.966	13.680	0.236	19.085	62.03	3	20	85.00	71.22
S16	3	5	60	8	52	15.385	21.400	0.412	29.155	60.47	2	16	87.50	71.28
S17	2	5	40	4	83	4.819	12.900	0.155	13.452	75.48	0	27	100.00	85.29
S18	0	5	0	0	44	0.000	0.000	0.000	0.000	100.00	0	16	100.00	100.00
S19	1	5	20	1	83	1.205	9.000	0.108	9.783	87.13	0	26	100.00	92.28
S20	3	5	60	3	128	2.344	4.680	0.037	3.527	65.27	0	40	100.00	79.16
S21	2	5	40	2	57	3.509	9.300	0.163	14.027	75.44	1	14	92.86	82.41
S22	3	5	60	7	30	23.333	11.647	0.388	27.965	59.48	0	10	100.00	75.69
S23	0	5	0	0	34	0.000	0.000	0.000	0.000	100.00	0	10	100.00	100.00
S24	0	5	0	0	34	0.000	0.000	0.000	0.000	100.00	0	10	100.00	100.00
S25	0	5	0	0	27	0.000	0.000	0.000	0.000	100.00	0	4	100.00	100.00
S26	0	5	0	0	29	0.000	0.000	0.000	0.000	100.00	0	6	100.00	100.00
S27	1	5	20	1	34	2.941	0.020	0.001	0.059	88.33	0	11	100.00	93.00
S28	1	5	20	2	34	5.882	10.000	0.294	22.727	82.19	0	14	100.00	89.32
S29	3	5	60	3	35	8.571	1.514	0.043	4.146	64.92	0	12	100.00	78.95
S30	2	5	40	2	30	6.667	1.233	0.041	3.949	76.48	0	8	100.00	85.89
S31	0	5	0	0	33	0.000	0.000	0.000	0.000	100.00	0	10	100.00	100.00
S32	3	5	60	4	43	9.302	3.747	0.087	8.015	64.64	0	10	100.00	78.78
S33	1	5	20	1	40	2.500	1.000	0.025	2.439	88.28	0	12	100.00	92.97
S34	0	5	0	0	43	0.000	0.000	0.000	0.000	100.00	0	15	100.00	100.00
S35	1	5	20	1	44	2.273	1.267	0.029	2.798	88.27	0	14	100.00	92.96
S36	4	5	80	12	54	22.222	12.239	0.227	18.477	50.89	0	18	100.00	70.53
S37	4	5	80	9	48	18.750	29.787	0.621	38.293	47.66	0	16	100.00	68.60

S38	4	5	80	7	58	12.069	23.528	0.406	28.859	50.41	1	22	95.45	68.42
S39	3	5	60	4	49	8.163	10.380	0.212	17.481	63.61	0	16	100.00	78.17
S40	1	5	20	3	113	2.655	3.000	0.027	2.586	88.26	2	42	95.24	91.05
S41	0	5	0	0	57	0.000	0.000	0.000	0.000	100.00	0	14	100.00	100.00
S42	2	5	40	3	44	6.818	1.673	0.038	3.664	76.48	0	16	100.00	85.89
S43	1	5	20	1	25	4.000	0.353	0.014	1.394	88.20	0	8	100.00	92.92
S44	4	5	80	10	39	25.641	14.663	0.376	27.325	48.99	0	14	100.00	69.40
S45	3	5	60	3	35	8.571	13.553	0.387	27.914	61.47	0	12	100.00	76.88
S46	0	5	0	0	24	0.000	0.000	0.000	0.000	100.00	0	4	100.00	100.00
S47	0	5	0	0	27	0.000	0.000	0.000	0.000	100.00	0	10	100.00	100.00
S48	3	5	60	7	128	5.469	5.253	0.041	3.942	65.14	3	48	93.75	76.58
S49	2	5	40	5	43	11.628	1.520	0.035	3.414	75.87	0	18	100.00	85.52
S50	0	5	0	0	29	0.000	0.000	0.000	0.000	100.00	0	6	100.00	100.00
S51	1	5	20	1	43	2.326	1.000	0.023	2.273	88.30	0	14	100.00	92.98
S52	0	5	0	0	30	0.000	0.000	0.000	0.000	100.00	0	8	100.00	100.00
S53	4	5	80	7	30	23.333	18.616	0.621	38.292	47.05	0	8	100.00	68.23
S54	4	5	80	14	34	41.176	24.640	0.725	42.019	42.67	0	10	100.00	65.60
S55	1	5	20	1	29	3.448	1.000	0.034	3.333	88.13	0	10	100.00	92.88
S56	4	5	80	18	48	37.500	41.809	0.871	46.553	42.34	0	18	100.00	65.40
S57	3	5	60	9	104	8.654	22.733	0.219	17.938	63.50	6	36	83.33	71.43
S58	1	5	20	2	28	7.143	2.000	0.071	6.667	87.15	2	8	75.00	82.29
S59	0	5	0	0	39	0.000	0.000	0.000	0.000	100.00	0	12	100.00	100.00
S60	0	5	0	0	24	0.000	0.000	0.000	0.000	100.00	0	4	100.00	100.00
S61	0	5	0	0	30	0.000	0.000	0.000	0.000	100.00	1	8	87.50	95.00
S62	1	5	20	1	34	2.941	9.000	0.265	20.930	83.20	0	10	100.00	89.92
S63	1	5	20	1	29	3.448	0.233	0.008	0.798	88.27	0	12	100.00	92.96
S64	1	5	20	1	38	2.632	9.000	0.237	19.149	83.94	0	10	100.00	90.36
S65	0	5	0	0	34	0.000	0.000	0.000	0.000	100.00	0	10	100.00	100.00
S66	2	5	40	2	33	6.061	3.373	0.102	9.274	76.04	0	12	100.00	85.62
S67	2	5	40	7	88	7.955	14.120	0.160	13.827	75.14	0	32	100.00	85.08
S68	0	5	0	0	40	0.000	0.000	0.000	0.000	100.00	0	16	100.00	100.00
S69	1	5	20	1	30	3.333	0.600	0.020	1.961	88.24	0	10	100.00	92.94
S70	0	5	0	0	32	0.000	0.000	0.000	0.000	100.00	0	10	100.00	100.00
S71	2	5	40	2	28	7.143	1.127	0.040	3.868	76.43	0	8	100.00	85.86
S72	1	5	20	3	30	10.000	0.433	0.014	1.424	87.06	0	10	100.00	92.24
S73	1	5	20	1	38	2.632	0.167	0.004	0.437	88.35	0	12	100.00	93.01
S74	1	5	20	1	34	2.941	1.000	0.029	2.857	88.21	0	10	100.00	92.93
S75	1	5	20	1	69	1.449	0.187	0.003	0.270	88.42	1	24	95.83	91.39
S76	0	5	0	0	28	0.000	0.000	0.000	0.000	100.00	0	6	100.00	100.00
S77	0	5	0	0	30	0.000	0.000	0.000	0.000	100.00	0	12	100.00	100.00
S78	0	5	0	0	35	0.000	0.000	0.000	0.000	100.00	0	12	100.00	100.00
S79	0	5	0	0	25	0.000	0.000	0.000	0.000	100.00	0	10	100.00	100.00
S80	0	5	0	0	34	0.000	0.000	0.000	0.000	100.00	0	10	100.00	100.00
S81	1	5	20	1	23	4.348	0.140	0.006	0.605	88.18	0	6	100.00	92.91
S82	1	5	20	1	34	2.941	0.240	0.007	0.701	88.32	0	8	100.00	92.99
S83	0	5	0	0	29	0.000	0.000	0.000	0.000	100.00	0	8	100.00	100.00

S84	1	5	20	1	29	3.448	9.000	0.310	23.684	81.99	0	10	100.00	89.20
S85	0	5	0	0	17	0.000	0.000	0.000	0.000	100.00	0	6	100.00	100.00
S86	0	5	0	0	30	0.000	0.000	0.000	0.000	100.00	0	8	100.00	100.00
S87	0	5	0	0	30	0.000	0.000	0.000	0.000	100.00	0	12	100.00	100.00
S88	1	5	20	1	33	3.030	1.000	0.030	2.941	88.20	0	12	100.00	92.92
S89	0	5	0	0	1289	0.000	0.000	0.000	0.000	100.00	1	404	99.75	99.90

¹Relative importance weights applied in the calculations: $W_1 = 0,6$ e $W_2 = 0,4$.

The resulting values (Tab. B2) were categorized into a range between 0 and 100, where 0 represents the 'worst' water quality and 100 represents the 'best' water quality [11,15], as shown in Table B3.

Table B3. Categorization scheme of the CCMEWQI_{Mod} index

Classification	WQI Value	Description
Excellent	95-100	Water quality is protected with a virtual absence of impairment; conditions are very close to pristine levels; these index values can only be obtained if all measurements meet recommended guidelines virtually all the time.
Very good	89-94	Water quality is protected with a slight presence of impairment; conditions are close to pristine levels.
Good	80-88	Water quality is protected with only a minor degree of impairment; conditions rarely depart from desirable levels.
Fair	65-79	Water quality is usually protected but occasionally impaired; conditions sometimes depart from desirable levels.
Marginal	45-64	Water quality is frequently impaired; conditions often depart from desirable levels.
Poor	0-44	Water quality is almost always impaired; conditions usually depart from desirable levels.

B.1.4. Geographic Information System (GIS)

The CCMEWQI_{Mod} was spatially represented in the distribution system using the QGIS software, allowing accurate estimates of water quality in areas where direct data were not available, through spatial interpolation distribution, helping to fill gaps in data coverage and identifying local problems. In addition, geoprocessing components and tools were used to extract water quality results in each pipe of the distribution network.

B.1.4.1. Spatial Interpolation Distribution

Among the spatial distribution methods [5], unlike geostatistical techniques [6], deterministic interpolation techniques create surfaces from measured points, based on the extent of similarity (for example, inverse distance interpolation) or the degree of smoothing (for example, radial basis functions) [7]. In this study, it was found that the inverse distance weighting (IDW) interpolation method was the most appropriate, as it only depended on the proximity of known points based on the principle that closer sample points have greater influence on the undetermined location. The calculation was performed by applying linear weighted combinations, as per equations 9 and 10 [8,19].

$$z = \frac{\sum_{i=1}^n x_i z_i}{\sum_{i=1}^n x_i} \quad (9)$$

$$x_i = \frac{1}{d_i^p} \quad (10)$$

Where: z is an unknown value for interpolation; z_i is the value of the data ($CCMEWQI_{Mod}$) "i" of the sampled location (S_i); n is the number of sampling points ($n = 89$); x_i is the weight for IDW analysis; d_i is the horizontal distance from the sample point to the estimated point; and p is the distance coefficient (equal to 3, because it is considered that the closest points have the greatest influence).

For datasets with a coefficient of variation less than 25%, the accuracy of IDW interpolation tends to increase using a higher "p" value ($2 \leq p \leq 4$) [20]. The processing of the $CCMEWQI_{Mod}$ interpolation was carried out using the "IDW interpolation" tool from QGIS, version 3.22.4-Białowieża, whose results were represented in Figure B2.

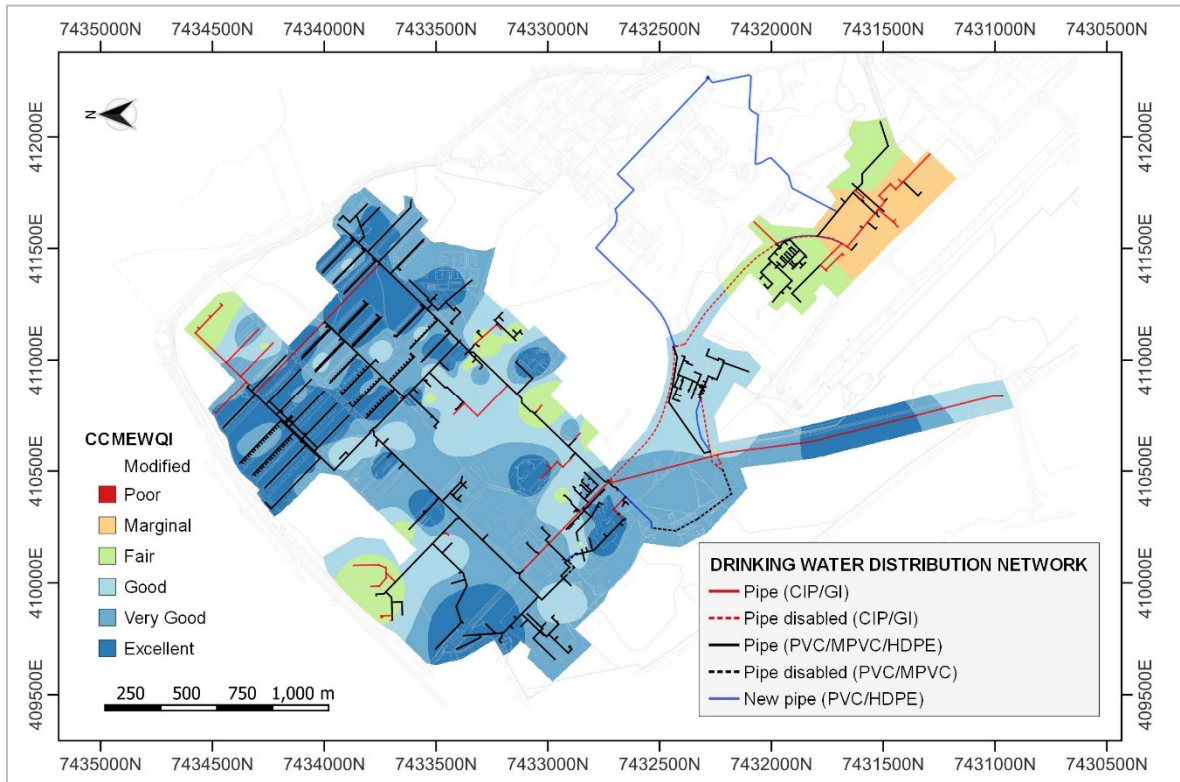


Figure B2. IDW Spatial Distribution of $CCMEWQI_{Mod}$

B.1.4.2. Geoprocessing

Geoprocessing tools were used to extract the water quality results in each section of the pipeline, using a simple field calculation in the attribute table of the respective vector layer, as per Equation 11.

$$CCMEWQI_{Pipe_i} = \frac{CCMEWQI_{Mod, Node_{start}} + CCMEWQI_{Mod, Node_{end}}}{2} \quad (11)$$

Where: The values of "CCME WQI_{Mod.Node}" were obtained from the raster layer produced in the IDW interpolation (Fig. B2)

After the geoprocessing was completed, the index value in each pipe of the distribution network is obtained, the results were represented in Figure B3.

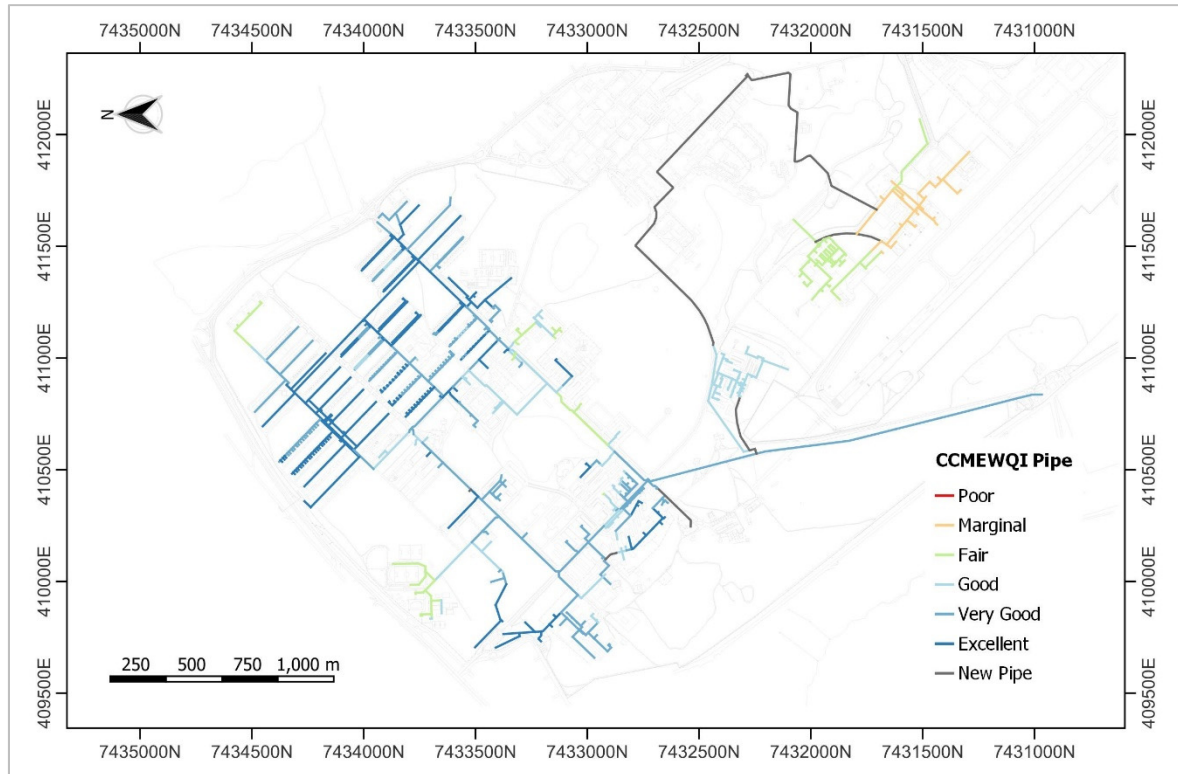


Figure B3. Value of CCMEWQI_{Mod} in the water distribution network.

References

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