water

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Article

Water quality modeling in headwater catchments: Comprehensive data assessments, model development and simulation of scenarios

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Supplementary Materials

S1. Univariate statistics for conventional water quality determinands

Table S1.1. Univariate statistics for conventional determinands in sub-basins S1 and S3.

Determinand (units)	Statistic	S1:1	S1:2	S1:3	S1:4	S3:1	S3:2	S3:3
Acidity (mg CaCO3/L)	Range	-	-	-	4.6 - 6	6 - 10.25	6 - 6	4.4 - 4.4
	Mean	-	-	-	5.533	8.038	6	4.4
	N (A, B) *	0 (0, 0)	0 (0, 0)	0 (0, 0)	3 (1, 2)	4 (2, 2)	4 (0, 4)	1 (1, 0)
Alkalinity (mg CaCO3/L)	Range	37.4 - 37.4	-	18.7 - 34.2	14.9 - 57.2	9.1 - 29	171 - 435	20.2 - 27.3
	Mean	37.4	-	26.45	27.217	17.82	238.8	23.75
	N (A, B)	1 (1, 0)	0 (0, 0)	2 (2, 0)	6 (6, 0)	5 (5, 0)	5 (5, 0)	2 (2, 0)
Bacteria: E Coli (MPN/100ml)	Range	-	100 - 3100	-	-	410 - 170000	130000 - 39000000	-
	Mean	-	788	-	-	37698.571	18447142.9	-
	N (A, B)	0 (0, 0)	5 (4, 1)	0 (0, 0)	0 (0, 0)	7 (7, 0)	7 (7, 0)	0 (0, 0)
Bacteria: E Coli (CFU/100ml)	Range	1800 - 1800	-	100 - 200	2000 - 2000	-	-	17000 - 48000
	Mean	1800	-	150	2000	-	-	32500
	N (A, B)	1 (1, 0)	0 (0, 0)	2 (2, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	2 (2, 0)
Bacteria: Tot. Coliforms (MPN/100ml)	Range	2000 - 2000	-	4500 - 4500	1200 - 50000	630 - 240000	240000 - 120000000	-
	Mean	2000	-	4500	15780	83761.429	63177142.9	-
	N (A, B)	1 (1, 0)	0 (0, 0)	1 (1, 0)	5 (5, 0)	7 (7, 0)	7 (7, 0)	0 (0, 0)
Bacteria: Tot. Coliforms (CFU/100ml)	Range	18000 - 18000	-	5400 - 8800	11000 - 11000	-	-	117000 - 129000
	Mean	18000	-	7100	11000	-	-	123000
	N (A, B)	1 (1, 0)	0 (0, 0)	2 (2, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	2 (2, 0)
BOD: 5 day Total (mgO2/L)	Range	2.8 - 2.8	-	3.6 - 4.2	1.5 - 8	2 - 7.8	4.8 - 441	5.4 - 7
	Mean	2.8	-	3.9	3.367	3.171	302.971	6.2
	N (A, B)	1 (1, 0)	0 (0, 0)	2 (2, 0)	6 (4, 2)	7 (3, 4)	7 (7, 0)	2 (2, 0)
BOD: 5 day Soluble (mgO2/L)	Range	2 - 2	-	1.1 - 2.2	3.2 - 3.2	2 - 7.6	94.3 - 315	1.6 - 1.6
	Mean	2	-	1.65	3.2	4.025	194.325	1.6
	N (A, B)	1 (1, 0)	0 (0, 0)	2 (2, 0)	1 (1, 0)	4 (3, 1)	4 (4, 0)	1 (1, 0)
BOD: 30 day (mgO2/L)	Range	-	-	-	3.4 - 3.4	-	-	16.6 - 16.6
	Mean	-	-	-	3.4	-	-	16.6
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)
Chlorophyll A (mg/m3)	Range	-	-	4 - 4	-	-	-	65 - 65
	Mean	-	-	4	-	-	-	65
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)
COD: Total	Range	14.7 - 14.7	-	18.7 - 21.8	10 - 73.1	10 - 61.4	24.7 - 1504	29.8 - 30

(mgO2/L)	Mean	14.7	-	20.25	29.15	25.571	675.714	29.9
	N (A, B)	1 (1, 0)	0 (0, 0)	2 (2, 0)	6 (5, 1)	7 (6, 1)	7 (7, 0)	2 (2, 0)
COD: Soluble (mgO2/L)	Range	10.5 - 10.5	-	9.9 - 14.1	-	14.9 - 52.7	124 - 255	15.7 - 15.7
	Mean	10.5	-	12	-	27.6	208	15.7
	N (A, B)	1 (1, 0)	0 (0, 0)	2 (2, 0)	0 (0, 0)	4 (4, 0)	3 (3, 0)	1 (1, 0)
Color (Pt/Co)	Range	-	-	-	20 - 60	14 - 40	19 - 130	40 - 40
	Mean	-	-	-	40	23.6	62.25	40
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	3 (3, 0)	5 (5, 0)	4 (4, 0)	1 (1, 0)
Conductivity (µS/cm)	Range	126.6 - 126.6	689 - 689	91.5 - 169.9	82.9 - 144	57.5 - 143	79.8 - 1336	91.8 - 118
	Mean	126.6	689	130.7	120.217	98.657	881.543	104.9
	N (A, B)	1 (1, 0)	1 (1, 0)	2 (2, 0)	6 (6, 0)	7 (7, 0)	7 (7, 0)	2 (2, 0)
Dissolved Oxygen (mg/L)	Range	3.85 - 3.85	4.67 - 4.67	2.65 - 6.01	0.6 - 5.2	4.6 - 7.5	0 - 5	3.7 - 5.2
	Mean	3.85	4.67	4.33	3.637	6.214	1.069	4.45
	N (A, B)	1 (1, 0)	1 (1, 0)	2 (2, 0)	6 (6, 0)	7 (7, 0)	7 (7, 0)	2 (2, 0)
Hardness: Ca (mg CaCO3/L)	Range	-	-	-	15 - 15	-	-	10 - 10
	Mean	-	-	-	15	-	-	10
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)
Hardness: Total (mg CaCO3/L)	Range	-	-	-	18 - 45.75	27.68 - 39.33	66.69 - 121.25	12 - 12
	Mean	-	-	-	36.44	33.733	94.44	12
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	5 (5, 0)	4 (4, 0)	4 (4, 0)	1 (1, 0)
N: Ammonia (mg/L)	Range	0.9 - 0.9	-	0.16 - 0.3	0.09 - 0.7	0.7 - 1.069	0.7 - 97.8	0.8 - 1.03
	Mean	0.9	-	0.23	0.598	0.753	41.339	0.915
	N (A, B)	1 (1, 0)	0 (0, 0)	2 (2, 0)	6 (1, 5)	7 (1, 6)	7 (6, 1)	2 (2, 0)
N: Nitrate (mg/L)	Range	0.44 - 0.44	-	0.11 - 0.97	0.279 - 1.2	0.19 - 0.575	0.1 - 1.04	0.11 - 0.8
	Mean	0.44	-	0.54	0.668	0.385	0.595	0.455
	N (A, B)	1 (1, 0)	0 (0, 0)	2 (1, 1)	6 (5, 1)	7 (6, 1)	7 (4, 3)	2 (0, 2)
N: Nitrite (mg/L)	Range	0.04 - 0.04	-	0.041 - 0.041	0.003 - 0.5	0.004 - 0.5	0.004 - 0.5	0.029 - 0.029
	Mean	0.04	-	0.041	0.112	0.167	0.197	0.029
	N (A, B)	1 (1, 0)	0 (0, 0)	1 (1, 0)	6 (3, 3)	7 (1, 6)	6 (2, 4)	1 (1, 0)
N: TKN (mg/L)	Range	1.3 - 1.3	-	0.9 - 1.1	0.9 - 1.2	1 - 1.3	31.3 - 140	1.7 - 2.1
	Mean	1.3	-	1	1.067	1.15	77.6	1.9
	N (A, B)	1 (1, 0)	0 (0, 0)	2 (1, 1)	3 (2, 1)	4 (3, 1)	4 (4, 0)	2 (2, 0)
N: Total (mg/L)	Range	-	-	-	1 - 2.4	0.19 - 1.45	50.6 - 140	-
	Mean	-	-	-	1.546	0.96	82.465	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	5 (3, 2)	4 (3, 1)	4 (4, 0)	0 (0, 0)
Oil & Grease (mg/L)	Range	-	-	3.6 - 3.6	8 - 39	10 - 95	10 - 52.4	3.6 - 9.5
	Mean	-	-	3.6	19.333	38.333	28.025	6.55
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (0, 1)	3 (2, 1)	3 (1, 2)	4 (2, 2)	2 (1, 1)
P: SRP (mg/L)	Range	0.13 - 0.13	-	0.01 - 0.15	0.023 - 1	0.01 - 1	3.46 - 19.09	0.01 - 0.13
	Mean	0.13	-	0.08	0.292	0.352	10.185	0.07
	N (A, B)	1 (1, 0)	0 (0, 0)	2 (1, 1)	5 (3, 2)	7 (3, 4)	4 (4, 0)	2 (1, 1)
P: Total (mg/L)	Range	0.38 - 0.38	-	0.17 - 0.33	0.06 - 2.191	0.06 - 0.188	0.165 - 14.926	0.16 - 0.24
	Mean	0.38	-	0.25	0.454	0.122	8.103	0.2
	N (A, B)	1 (1, 0)	0 (0, 0)	2 (2, 0)	6 (4, 2)	7 (6, 1)	7 (7, 0)	2 (2, 0)
pH (pH)	Range	6.83 - 6.83	4.42 - 4.42	6.25 - 6.53	6.25 - 7.31	6.3 - 7.5	6.9 - 8.33	6.23 - 6.76
	Mean	6.83	4.42	6.39	6.782	7.14	7.521	6.495
	N (A, B)	1 (1, 0)	1 (1, 0)	2 (2, 0)	6 (6, 0)	7 (7, 0)	7 (7, 0)	2 (2, 0)
Streamflow (m3/s)	Range	0.174 - 0.174	-	0.076 - 2.332	0.264 - 0.698	0.112 - 0.48	0.001 - 0.006	0.252 - 0.448
	Mean	0.174	-	1.204	0.487	0.296	0.003	0.35
	N (A, B)	1 (1, 0)	0 (0, 0)	2 (2, 0)	4 (4, 0)	2 (2, 0)	4 (4, 0)	2 (2, 0)
Solids: Dissolved (mg/L)	Range	-	-	67 - 67	-	-	-	62 - 62
	Mean	-	-	67	-	-	-	62

	N (A, B)	0 (0, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)
Solids: Sedimentable (mg/L)	Range	-	-	-	-	-	-	-
	Mean	-	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
Solids Total (mg/L)	Range	130 - 130	-	158 - 158	76 - 174	53 - 264	603 - 1036	110 - 110
	Mean	130	-	158	109.333	116.717	807.833	110
	N (A, B)	1 (1, 0)	0 (0, 0)	1 (1, 0)	6 (6, 0)	6 (6, 0)	6 (6, 0)	1 (1, 0)
Solids: Total Suspended (mg/L)	Range	10 - 10	-	15 - 29	4 - 40	5.5 - 144	27 - 673	14 - 18
	Mean	10	-	22	16.167	47.957	298.143	16
	N (A, B)	1 (1, 0)	0 (0, 0)	2 (2, 0)	6 (5, 1)	7 (7, 0)	7 (7, 0)	2 (2, 0)
Solids: Volatile Suspended (mg/L)	Range	2.6 - 2.6	-	4.3 - 7	-	-	-	5.7 - 5.7
	Mean	2.6	-	5.65	-	-	-	5.7
	N (A, B)	1 (1, 0)	0 (0, 0)	2 (2, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)
Surfactants (mg/L)	Range	-	-	-	0.03 - 0.1	0.16 - 0.4	0.4 - 6.76	0.22 - 0.22
	Mean	-	-	-	0.065	0.352	3.786	0.22
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	2 (1, 1)	5 (1, 4)	5 (4, 1)	1 (1, 0)
Temperature: Air (°C)	Range	25 - 25	25 - 25	23 - 28.6	16.8 - 21.5	15.8 - 23.2	16 - 17.9	22.5 - 22.5
	Mean	25	25	25.8	19.65	18.45	16.925	22.5
	N (A, B)	1 (1, 0)	1 (1, 0)	2 (2, 0)	4 (4, 0)	4 (4, 0)	4 (4, 0)	1 (1, 0)
Temperature: Water (°C)	Range	17.3 - 17.3	16.5 - 16.5	14.9 - 18.5	13.9 - 17.5	12.8 - 14.7	14.8 - 18.2	13.91 - 14.7
	Mean	17.3	16.5	16.7	16.152	13.667	17.05	14.305
	N (A, B)	1 (1, 0)	1 (1, 0)	2 (2, 0)	6 (6, 0)	6 (6, 0)	6 (6, 0)	2 (2, 0)
TOC (mg/L)	Range	-	-	-	9.2 - 9.91	9.3 - 9.3	167 - 167	-
	Mean	-	-	-	9.555	9.3	167	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	2 (2, 0)	1 (1, 0)	1 (1, 0)	0 (0, 0)
Turbidity (NTU)	Range	-	-	-	5.9 - 69.4	7.6 - 71.5	128 - 253	17.8 - 17.8
	Mean	-	-	-	22.85	33.64	202	17.8
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	6 (6, 0)	5 (5, 0)	5 (5, 0)	1 (1, 0)

* N: Number of records; A & B: Number of records above and below detection limits.

Table S1.2. Univariate statistics for conventional determinands in sub-basins S4 and S5.

Determinand (units)	Statistic	S4:1	S4:2	S4:3	S4:4	S4:5	S5:1
Acidity (mg CaCO3/L)	Range	6 - 6	27.2 - 27.2	10.6 - 10.6	26.3 - 26.3	319 - 319	-
	Mean	6	27.2	10.6	26.3	319	-
	N (A, B) *	1 (0, 1)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	0 (0, 0)
Alkalinity (mg CaCO3/L)	Range	-	5 - 5	12.8 - 12.8	6.5 - 6.5	-	146 - 146
	Mean	-	5	12.8	6.5	-	146
	N (A, B)	0 (0, 0)	1 (0, 1)	1 (1, 0)	1 (1, 0)	0 (0, 0)	1 (1, 0)
Bacteria: E Coli (MPN/100ml)	Range	-	-	5800 - 5800	1100 - 1100	-	-
	Mean	-	-	5800	1100	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (1, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)
Bacteria: E Coli (CFU/100ml)	Range	-	-	-	-	-	6000 - 6000
	Mean	-	-	-	-	-	6000
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)
Bacteria: Tot. Coliforms (MPN/100ml)	Range	-	-	560 - 560	86 - 86	-	-
	Mean	-	-	560	86	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (1, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)
Bacteria: Tot. Coliforms (CFU/100ml)	Range	-	-	-	-	-	66000 - 66000
	Mean	-	-	-	-	-	66000
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)
BOD: 5 day Total	Range	3.2 - 3.2	2 - 2	2 - 2	2 - 2	11 - 11	3.89 - 3.89

(mgO2/L)	Mean	3.2	2	2	2	11	3.89
	N (A, B)	1 (1, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (1, 0)	1 (1, 0)
BOD: 5 day Soluble (mgO2/L)	Range	-	-	-	-	-	1 - 1
	Mean	-	-	-	-	-	1
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (0, 1)
BOD: 30 day (mgO2/L)	Range	-	-	-	-	-	-
	Mean	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
Chlorophyll A (mg/m3)	Range	-	-	-	-	-	-
	Mean	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
COD: Total (mgO2/L)	Range	10 - 10	16.3 - 16.3	10 - 10	77.69 - 77.69	21.7 - 21.7	219 - 219
	Mean	10	16.3	10	77.69	21.7	219
	N (A, B)	1 (0, 1)	1 (1, 0)	1 (0, 1)	1 (1, 0)	1 (1, 0)	1 (1, 0)
COD: Soluble (mgO2/L)	Range	-	-	-	-	-	3.27 - 3.27
	Mean	-	-	-	-	-	3.27
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)
Color (Pt/Co)	Range	3 - 3	5 - 5	40 - 40	40 - 40	10 - 10	5 - 5
	Mean	3	5	40	40	10	5
	N (A, B)	1 (0, 1)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)
Conductivity (µS/cm)	Range	-	687 - 687	52.3 - 52.3	63.3 - 63.3	2340 - 2340	-
	Mean	-	687	52.3	63.3	2340	-
	N (A, B)	0 (0, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	0 (0, 0)
Dissolved Oxygen (mg/L)	Range	-	3.3 - 3.3	4.45 - 4.45	4.94 - 4.94	2.8 - 2.8	-
	Mean	-	3.3	4.45	4.94	2.8	-
	N (A, B)	0 (0, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	0 (0, 0)
Hardness: Ca (mg CaCO3/L)	Range	-	137 - 137	9.29 - 9.29	9.39 - 9.39	704 - 704	-
	Mean	-	137	9.29	9.39	704	-
	N (A, B)	0 (0, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	0 (0, 0)
Hardness: Total (mg CaCO3/L)	Range	89.2 - 89.2	284 - 284	10.65 - 10.65	10.78 - 10.78	1137 - 1137	-
	Mean	89.2	284	10.65	10.78	1137	-
	N (A, B)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	0 (0, 0)
N: Ammonia (mg/L)	Range	0.7 - 0.7	0.7 - 0.7	0.7 - 0.7	0.7 - 0.7	5 - 5	0.43 - 0.43
	Mean	0.7	0.7	0.7	0.7	5	0.43
	N (A, B)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (1, 0)	1 (1, 0)
N: Nitrate (mg/L)	Range	0.359 - 0.359	0.1 - 0.1	0.113 - 0.113	0.113 - 0.113	0.1 - 0.1	0.11 - 0.11
	Mean	0.359	0.1	0.113	0.113	0.1	0.11
	N (A, B)	1 (1, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)
N: Nitrite (mg/L)	Range	0.005 - 0.005	0.004 - 0.004	0.152 - 0.152	0.152 - 0.152	0.004 - 0.004	-
	Mean	0.005	0.004	0.152	0.152	0.004	-
	N (A, B)	1 (1, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	0 (0, 0)
N: TKN (mg/L)	Range	2.5 - 2.5	1 - 1	1 - 1	1.77 - 1.77	5.07 - 5.07	3.4 - 3.4
	Mean	2.5	1	1	1.77	5.07	3.4
	N (A, B)	1 (1, 0)	1 (0, 1)	1 (0, 1)	1 (1, 0)	1 (1, 0)	1 (1, 0)
N: Total (mg/L)	Range	-	-	0 - 0	1.77 - 1.77	5.07 - 5.07	-
	Mean	-	-	0	1.77	5.07	-
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	0 (0, 0)
Oil & Grease (mg/L)	Range	10 - 10	10 - 10	10 - 10	10 - 10	10 - 10	5.2 - 5.2
	Mean	10	10	10	10	10	5.2
	N (A, B)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (1, 0)
P: SRP (mg/L)	Range	0.01 - 0.01	-	0.326 - 0.326	0.326 - 0.326	-	0.02 - 0.02
	Mean	0.01	-	0.326	0.326	-	0.02

	N (A, B)	1 (0, 1)	0 (0, 0)	1 (0, 1)	1 (0, 1)	0 (0, 0)	1 (0, 1)
P: Total (mg/L)	Range	0.06 - 0.06	0.06 - 0.06	0.06 - 0.06	0.576 - 0.576	1.557 - 1.557	0.89 - 0.89
	Mean	0.06	0.06	0.06	0.576	1.557	0.89
	N (A, B)	1 (0, 1)	1 (1, 0)	1 (0, 1)	1 (1, 0)	1 (1, 0)	1 (1, 0)
pH (pH)	Range	7.11 - 7.11	4.4 - 4.4	6.55 - 6.55	6.67 - 6.67	3.92 - 3.92	-
	Mean	7.11	4.4	6.55	6.67	3.92	-
	N (A, B)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	0 (0, 0)
Streamflow (m3/s)	Range	-	0.002 - 0.002	-	-	-	-
	Mean	-	0.002	-	-	-	-
	N (A, B)	0 (0, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
Solids: Dissolved (mg/L)	Range	-	-	-	-	-	-
	Mean	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
Solids: Sedimentable (mg/L)	Range	0.1 - 0.1	0.1 - 0.1	0.1 - 0.1	1 - 1	0.1 - 0.1	-
	Mean	0.1	0.1	0.1	1	0.1	-
	N (A, B)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (1, 0)	1 (0, 1)	0 (0, 0)
Solids Total (mg/L)	Range	-	-	-	-	-	-
	Mean	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
Solids: Total Suspended (mg/L)	Range	7 - 7	7 - 7	6 - 6	214 - 214	28 - 28	420 - 420
	Mean	7	7	6	214	28	420
	N (A, B)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)
Solids: Volatile Suspended (mg/L)	Range	-	-	-	-	-	60 - 60
	Mean	-	-	-	-	-	60
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)
Surfactants (mg/L)	Range	0.4 - 0.4	0.4 - 0.4	0.4 - 0.4	0.4 - 0.4	0.4 - 0.4	0.02 - 0.02
	Mean	0.4	0.4	0.4	0.4	0.4	0.02
	N (A, B)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)
Temperature: Air (°C)	Range	15.2 - 15.2	12.1 - 12.1	16.3 - 16.3	16.9 - 16.9	12.9 - 12.9	-
	Mean	15.2	12.1	16.3	16.9	12.9	-
	N (A, B)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	0 (0, 0)
Temperature: Water (°C)	Range	16.7 - 16.7	14.6 - 14.6	13.7 - 13.7	15.8 - 15.8	18.3 - 18.3	-
	Mean	16.7	14.6	13.7	15.8	18.3	-
	N (A, B)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	0 (0, 0)
TOC (mg/L)	Range	-	-	-	-	-	-
	Mean	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
Turbidity (NTU)	Range	-	-	5.53 - 5.53	185 - 185	-	1379 - 1379
	Mean	-	-	5.53	185	-	1379
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (1, 0)	1 (1, 0)	0 (0, 0)	1 (1, 0)

* N: Number of records; A & B: Number of records above and below detection limits.

Table S1.3. Univariate statistics for conventional determinands in sub-basin S2: Part 1.

Determinand (units)	Statistic	S2:1	S2:2	S2:3	S2:4	S2:5	S2:6
Acidity (mg CaCO3/L)	Range	3.5 - 3.5	-	-	-	-	4.8 - 32.14
	Mean	3.5	-	-	-	-	16.835
	N (A, B) *	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	4 (3, 1)
Alkalinity (mg CaCO3/L)	Range	0.5 - 4.6	3.9 - 3.9	6.2 - 6.2	17.3 - 17.3	13.8 - 13.8	5 - 27.1
	Mean	2.55	3.9	6.2	17.3	13.8	11.371
	N (A, B)	2 (1, 1)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	7 (6, 1)
Bacteria: E Coli	Range	1 - 1	-	-	-	-	10 - 1000

(MPN/100ml)	Mean	1	-	-	-	-	388.333
	N (A, B)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	6 (4, 2)
Bacteria: E Coli (CFU/100ml)	Range	100 - 200	100 - 100	100 - 100	100 - 100	100 - 100	100 - 1000
	Mean	150	100	100	100	100	533.333
	N (A, B)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	3 (3, 0)
Bacteria: Tot. Coliforms (MPN/100ml)	Range	-	-	4500 - 4500	2000 - 2000	2000 - 2000	440 - 11000
	Mean	-	-	4500	2000	2000	5720
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	7 (7, 0)
Bacteria: Tot. Coliforms (CFU/100ml)	Range	800 - 1000	2100 - 2100	4800 - 4800	6500 - 6500	5600 - 5600	3800 - 23000
	Mean	900	2100	4800	6500	5600	13600
	N (A, B)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	3 (3, 0)
BOD: 5 day Total (mgO2/L)	Range	2.5 - 3.5	3.7 - 3.7	2.2 - 2.2	1.7 - 1.7	1.4 - 1.4	2 - 3.3
	Mean	3	3.7	2.2	1.7	1.4	2.233
	N (A, B)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	9 (3, 6)
BOD: 5 day Soluble (mgO2/L)	Range	2.8 - 2.8	2.9 - 2.9	2.2 - 2.2	1.5 - 1.5	1.1 - 1.1	1 - 2
	Mean	2.8	2.9	2.2	1.5	1.1	1.72
	N (A, B)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	5 (1, 4)
BOD: 30 day (mgO2/L)	Range	4.3 - 4.3	-	-	-	-	6.6 - 6.6
	Mean	4.3	-	-	-	-	6.6
	N (A, B)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)
Chlorophyll A (mg/m3)	Range	4 - 4	3.8 - 3.8	-	-	-	1 - 1
	Mean	4	3.8	-	-	-	1
	N (A, B)	1 (1, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (0, 1)
COD: Total (mgO2/L)	Range	16 - 21.5	19.3 - 19.3	41.4 - 41.4	19.3 - 19.3	12.7 - 12.7	12.7 - 115
	Mean	18.75	19.3	41.4	19.3	12.7	32.322
	N (A, B)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	9 (9, 0)
COD: Soluble (mgO2/L)	Range	10.3 - 10.3	12 - 12	14.9 - 14.9	1.16 - 1.16	1.16 - 1.16	10 - 85.25
	Mean	10.3	12	14.9	1.16	1.16	27.81
	N (A, B)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (0, 1)	1 (0, 1)	5 (4, 1)
Color (Pt/Co)	Range	40 - 40	-	-	-	-	10 - 55
	Mean	40	-	-	-	-	27.2
	N (A, B)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	5 (5, 0)
Conductivity (µS/cm)	Range	21.2 - 31.8	30.6 - 30.6	144.8 - 144.8	264 - 264	213.2 - 213.2	53.8 - 215.3
	Mean	26.5	30.6	144.8	264	213.2	112.233
	N (A, B)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	9 (9, 0)
Dissolved Oxygen (mg/L)	Range	7.04 - 7.2	7.08 - 7.08	6.48 - 6.48	5.67 - 5.67	4.91 - 4.91	5.04 - 7.1
	Mean	7.12	7.08	6.48	5.67	4.91	6.442
	N (A, B)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	9 (9, 0)
Hardness: Ca (mg CaCO3/L)	Range	1 - 1	-	-	-	-	17.69 - 19.5
	Mean	1	-	-	-	-	18.595
	N (A, B)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	2 (2, 0)
Hardness: Total (mg CaCO3/L)	Range	1 - 1	-	-	-	-	27.5 - 35.66
	Mean	1	-	-	-	-	32.364
	N (A, B)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	5 (5, 0)
N: Ammonia (mg/L)	Range	0.14 - 0.3	0.2 - 0.2	0.12 - 0.12	0.2 - 0.2	0.2 - 0.2	0.06 - 0.7
	Mean	0.22	0.2	0.12	0.2	0.2	0.526
	N (A, B)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	9 (3, 6)
N: Nitrate (mg/L)	Range	0.11 - 0.8	0.11 - 0.11	0.53 - 0.53	0.31 - 0.31	0.31 - 0.31	0.1 - 0.9
	Mean	0.455	0.11	0.53	0.31	0.31	0.433
	N (A, B)	2 (0, 2)	1 (0, 1)	1 (1, 0)	1 (1, 0)	1 (1, 0)	9 (4, 5)
N: Nitrite (mg/L)	Range	0.002 - 0.002	-	0.002 - 0.002	0.002 - 0.002	0.002 - 0.002	0.002 - 0.5
	Mean	0.002	-	0.002	0.002	0.002	0.147

	N (A, B)	1 (0, 1)	0 (0, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)	8 (2, 6)
N: TKN (mg/L)	Range	0.9 - 0.9	0.9 - 0.9	0.9 - 0.9	0.9 - 0.9	0.9 - 0.9	0.9 - 1.1
	Mean	0.9	0.9	0.9	0.9	0.9	0.983
	N (A, B)	2 (0, 2)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	6 (1, 5)
N: Total (mg/L)	Range	-	-	-	-	-	0.3 - 1
	Mean	-	-	-	-	-	0.65
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	2 (1, 1)
Oil & Grease (mg/L)	Range	4 - 9.7	3.6 - 3.6	-	-	-	3.6 - 21.4
	Mean	6.85	3.6	-	-	-	11.98
	N (A, B)	2 (2, 0)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	5 (2, 3)
P: SRP (mg/L)	Range	0.01 - 0.01	0.01 - 0.01	0.2 - 0.2	0.09 - 0.09	0.11 - 0.11	0.01 - 1
	Mean	0.01	0.01	0.2	0.09	0.11	0.299
	N (A, B)	2 (0, 2)	1 (0, 1)	1 (1, 0)	1 (1, 0)	1 (1, 0)	9 (4, 5)
P: Total (mg/L)	Range	0.02 - 0.02	0.02 - 0.02	0.46 - 0.46	0.53 - 0.53	0.32 - 0.32	0.02 - 0.48
	Mean	0.02	0.02	0.46	0.53	0.32	0.123
	N (A, B)	2 (0, 2)	1 (0, 1)	1 (1, 0)	1 (1, 0)	1 (1, 0)	9 (3, 6)
pH (pH)	Range	4.9 - 4.94	5.05 - 5.05	5.8 - 5.8	6.22 - 6.22	6.19 - 6.19	5.93 - 7.09
	Mean	4.92	5.05	5.8	6.22	6.19	6.391
	N (A, B)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	9 (9, 0)
Streamflow (m3/s)	Range	0.01 - 0.052	-	0.003 - 0.003	-	0.006 - 0.006	0.077 - 0.646
	Mean	0.031	-	0.003	-	0.006	0.334
	N (A, B)	2 (2, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	1 (1, 0)	3 (3, 0)
Solids: Dissolved (mg/L)	Range	34 - 34	30 - 30	-	-	-	61 - 61
	Mean	34	30	-	-	-	61
	N (A, B)	1 (1, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)
Solids: Sedimentable (mg/L)	Range	-	-	-	-	-	-
	Mean	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
Solids Total (mg/L)	Range	42 - 42	-	196 - 196	294 - 294	221 - 221	80 - 292
	Mean	42	-	196	294	221	119.9
	N (A, B)	1 (1, 0)	0 (0, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	7 (7, 0)
Solids: Total Suspended (mg/L)	Range	7.4 - 10	7.8 - 7.8	18 - 18	69 - 69	22 - 22	4 - 59
	Mean	8.7	7.8	18	69	22	20.722
	N (A, B)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	9 (9, 0)
Solids: Volatile Suspended (mg/L)	Range	4 - 4	3.8 - 3.8	4.3 - 4.3	10 - 10	4.8 - 4.8	10 - 11
	Mean	4	3.8	4.3	10	4.8	10.5
	N (A, B)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	2 (2, 0)
Surfactants (mg/L)	Range	0.02 - 0.02	-	-	-	-	0.08 - 0.51
	Mean	0.02	-	-	-	-	0.304
	N (A, B)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	5 (3, 2)
Temperature: Air (°C)	Range	19 - 19	23.8 - 23.8	24.8 - 24.8	30 - 30	27 - 27	16.9 - 28.9
	Mean	19	23.8	24.8	30	27	21.1
	N (A, B)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	6 (6, 0)
Temperature: Water (°C)	Range	11.04 - 13.5	14.2 - 14.2	16.6 - 16.6	18.2 - 18.2	18 - 18	12 - 16.1
	Mean	12.27	14.2	16.6	18.2	18	13.919
	N (A, B)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	9 (9, 0)
TOC (mg/L)	Range	12.46 - 12.46	-	-	-	-	-
	Mean	12.46	-	-	-	-	-
	N (A, B)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
Turbidity (NTU)	Range	6.31 - 6.31	-	-	-	-	8.85 - 20.9
	Mean	6.31	-	-	-	-	14.95
	N (A, B)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	5 (5, 0)

Table S1.4. Univariate statistics for conventional determinands in sub-basin S2: Part 2.

Determinand (units)	Statistic	S1:1	S1:2	S1:3	S1:4	S3:1	S3:2	S3:3
Acidity (mg CaCO3/L)	Range	35.39 - 35.39	29 - 29	444 - 666	354 - 354	6 - 6	6 - 6	6 - 6
	Mean	35.39	29	555	354	6	6	6
	N (A, B) *	1 (1, 0)	1 (1, 0)	2 (2, 0)	1 (1, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)
Alkalinity (mg CaCO3/L)	Range	-	-	-	-	118 - 118	126 - 126	127 - 127
	Mean	-	-	-	-	118	126	127
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)
Bacteria: E Coli (MPN/100ml)	Range	-	1 - 1	-	1 - 1	100 - 100	200 - 200	100 - 100
	Mean	-	1	-	1	100	200	100
	N (A, B)	0 (0, 0)	1 (0, 1)	0 (0, 0)	1 (0, 1)	1 (1, 0)	1 (1, 0)	1 (0, 1)
Bacteria: E Coli (CFU/100ml)	Range	-	-	-	-	-	-	-
	Mean	-	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
Bacteria: Tot. Coliforms (MPN/100ml)	Range	-	2 - 2	1 - 1	1 - 1	4800 - 4800	5500 - 5500	3500 - 3500
	Mean	-	2	1	1	4800	5500	3500
	N (A, B)	0 (0, 0)	1 (1, 0)	1 (0, 1)	1 (0, 1)	1 (1, 0)	1 (1, 0)	1 (1, 0)
Bacteria: Tot. Coliforms (CFU/100ml)	Range	-	-	-	-	-	-	-
	Mean	-	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
BOD: 5 day Total (mgO2/L)	Range	3.6 - 3.6	2 - 2	23.4 - 33.3	19 - 19	2.1 - 2.1	2 - 2	2 - 2
	Mean	3.6	2	28.35	19	2.1	2	2
	N (A, B)	1 (1, 0)	1 (0, 1)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (0, 1)	1 (0, 1)
BOD: 5 day Soluble (mgO2/L)	Range	-	-	-	-	-	-	-
	Mean	-	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
BOD: 30 day (mgO2/L)	Range	-	-	-	-	-	-	-
	Mean	-	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
Chlorophyll A (mg/m3)	Range	-	-	-	-	-	-	-
	Mean	-	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
COD: Total (mgO2/L)	Range	160 - 160	11.7 - 11.7	34.4 - 187	37.6 - 37.6	16.4 - 16.4	10 - 10	10.7 - 10.7
	Mean	160	11.7	110.7	37.6	16.4	10	10.7
	N (A, B)	1 (1, 0)	1 (1, 0)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (0, 1)	1 (1, 0)
COD: Soluble (mgO2/L)	Range	-	-	-	-	-	-	-
	Mean	-	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
Color (Pt/Co)	Range	2.5 - 2.5	3 - 3	10 - 40	10 - 10	19 - 19	19 - 19	16 - 16
	Mean	2.5	3	25	10	19	19	16
	N (A, B)	1 (1, 0)	1 (1, 0)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)
Conductivity (µS/cm)	Range	232 - 232	228 - 228	1187 - 1541	1120 - 1120	248 - 248	249 - 249	285 - 285
	Mean	232	228	1364	1120	248	249	285
	N (A, B)	1 (1, 0)	1 (1, 0)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)
Dissolved Oxygen (mg/L)	Range	4.6 - 4.6	5.6 - 5.6	4.7 - 5.5	5.2 - 5.2	2.49 - 2.49	6.58 - 6.58	6.21 - 6.21
	Mean	4.6	5.6	5.1	5.2	2.49	6.58	6.21
	N (A, B)	1 (1, 0)	1 (1, 0)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)
Hardness: Ca (mg CaCO3/L)	Range	25.62 - 25.62	-	108.27 - 108.27	-	29.34 - 29.34	-	36.46 - 36.46
	Mean	25.62	-	108.27	-	29.34	-	36.46
	N (A, B)	1 (1, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	1 (1, 0)
Hardness: Total	Range	62.1 - 62.1	-	231 - 231	-	44.38 - 44.38	-	60.73 - 60.73

(mg CaCO3/L)	Mean	62.1	-	231	-	44.38	-	60.73
	N (A, B)	1 (1, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	1 (1, 0)
N: Ammonia (mg/L)	Range	0.7 - 0.7	0.7 - 0.7	0.7 - 0.7	0.7 - 0.7	0.7 - 0.7	0.7 - 0.7	0.7 - 0.7
	Mean	0.7	0.7	0.7	0.7	0.7	0.7	0.7
	N (A, B)	1 (0, 1)	1 (0, 1)	2 (0, 2)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)
N: Nitrate (mg/L)	Range	0.14 - 0.14	0.1 - 0.1	0.1 - 0.5	0.1 - 0.1	0.38 - 0.38	0.3 - 0.3	0.57 - 0.57
	Mean	0.14	0.1	0.3	0.1	0.38	0.3	0.57
	N (A, B)	1 (1, 0)	1 (0, 1)	2 (0, 2)	1 (0, 1)	1 (1, 0)	1 (1, 0)	1 (1, 0)
N: Nitrite (mg/L)	Range	0.5 - 0.5	0.004 - 0.004	0.006 - 0.5	0.004 - 0.004	0.152 - 0.152	0.152 - 0.152	0.152 - 0.152
	Mean	0.5	0.004	0.253	0.004	0.152	0.152	0.152
	N (A, B)	1 (0, 1)	1 (0, 1)	2 (1, 1)	1 (1, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)
N: TKN (mg/L)	Range	1.9 - 1.9	-	5 - 5	-	1 - 1	1 - 1	1 - 1
	Mean	1.9	-	5	-	1	1	1
	N (A, B)	1 (1, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)
N: Total (mg/L)	Range	2.04 - 2.04	1 - 1	1.3 - 5	1.7 - 1.7	0.38 - 0.38	0.3 - 0.3	0.57 - 0.57
	Mean	2.04	1	3.15	1.7	0.38	0.3	0.57
	N (A, B)	1 (1, 0)	1 (0, 1)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)
Oil & Grease (mg/L)	Range	32.5 - 32.5	10 - 10	10 - 11	10 - 10	10 - 10	10 - 10	10 - 10
	Mean	32.5	10	10.5	10	10	10	10
	N (A, B)	1 (1, 0)	1 (0, 1)	2 (0, 2)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)
P: SRP (mg/L)	Range	-	-	-	-	0.326 - 0.326	0.326 - 0.326	0.326 - 0.326
	Mean	-	-	-	-	0.326	0.326	0.326
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)
P: Total (mg/L)	Range	0.746 - 0.746	0.06 - 0.06	0.06 - 2.597	0.114 - 0.114	0.115 - 0.115	0.098 - 0.098	0.078 - 0.078
	Mean	0.746	0.06	1.329	0.114	0.115	0.098	0.078
	N (A, B)	1 (1,)	1 (0, 1)	2 (1, 1)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)
pH (pH)	Range	4.2 - 4.2	4 - 4	3.2 - 3.3	3.1 - 3.1	8.18 - 8.18	8.35 - 8.35	7.83 - 7.83
	Mean	4.2	4	3.25	3.1	8.18	8.35	7.83
	N (A, B)	1 (1, 0)	1 (1, 0)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)
Streamflow (m3/s)	Range	0 - 0	-	0.002 - 0.002	-	-	-	-
	Mean	0	-	0.002	-	-	-	-
	N (A, B)	1 (1, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
Solids: Dissolved (mg/L)	Range	-	-	-	-	-	-	-
	Mean	-	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
Solids: Sedimentable (mg/L)	Range	1.5 - 1.5	0.1 - 0.1	0.1 - 27	0.1 - 0.1	0.1 - 0.1	0.1 - 0.1	0.1 - 0.1
	Mean	1.5	0.1	13.55	0.1	0.1	0.1	0.1
	N (A, B)	1 (1, 0)	1 (0, 1)	2 (1, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)
Solids Total (mg/L)	Range	-	-	-	-	-	-	-
	Mean	-	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
Solids: Total Suspended (mg/L)	Range	500 - 500	19 - 19	455 - 455	370 - 370	17 - 17	14 - 14	14.5 - 14.5
	Mean	500	19	455	370	17	14	14.5
	N (A, B)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)
Solids: Volatile Suspended (mg/L)	Range	-	-	-	-	-	-	-
	Mean	-	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
Surfactants (mg/L)	Range	0.1 - 0.1	0.4 - 0.4	0.1 - 0.4	0.4 - 0.4	0.4 - 0.4	0.4 - 0.4	0.4 - 0.4
	Mean	0.1	0.4	0.25	0.4	0.4	0.4	0.4
	N (A, B)	1 (0, 1)	1 (0, 1)	2 (0, 2)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)
Temperature: Air (°C)	Range	15 - 15	17.4 - 17.4	15.8 - 16.4	17.7 - 17.7	19.6 - 19.6	17.8 - 17.8	20.3 - 20.3
	Mean	15	17.4	16.1	17.7	19.6	17.8	20.3

	N (A, B)	1 (1, 0)	1 (1, 0)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)
Temperature: Water (°C)	Range	12.8 - 12.8	10.4 - 10.4	13.5 - 14.5	15.1 - 15.1	16 - 16	15.4 - 15.4	15.6 - 15.6
	Mean	12.8	10.4	14	15.1	16	15.4	15.6
	N (A, B)	1 (1, 0)	1 (1, 0)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)
TOC (mg/L)	Range	-	-	-	-	-	-	-
	Mean	-	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
Turbidity (NTU)	Range	-	-	-	-	24.3 - 24.3	21.8 - 21.8	24.8 - 24.8
	Mean	-	-	-	-	24.3	21.8	24.8
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)

* N: Number of records; A & B: Number of records above and below detection limits.

S2. Univariate statistics for toxic water quality determinands

Table S2.1. Univariate statistics for toxic determinands in sub-basins S1 and S3.

Toxicant (mg/L)	Statistic	S1:1	S1:2	S1:3	S1:4	S3:1	S3:2	S3:3
Ag	Range	-	-	0.033 - 0.033	0.002 - 0.011	0.002 - 0.011	0.002 - 0.011	0.002 - 0.033
	Mean	-	-	0.033	0.006	0.007	0.008	0.018
	N (A, B) *	0 (0, 0)	0 (0, 0)	1 (0, 1)	5 (1, 4)	5 (1, 4)	5 (1, 4)	2 (0, 2)
Al	Range	-	-	0.224 - 0.224	0.236 - 1.125	0.083 - 1.29	0.458 - 1.641	0.102 - 0.236
	Mean	-	-	0.224	0.502	0.555	1.099	0.169
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (1, 0)	5 (4, 1)	4 (4, 0)	4 (4, 0)	2 (1, 1)
As	Range	-	-	0.033 - 0.033	0.003 - 0.011	0.003 - 0.011	0.003 - 0.011	0.005 - 0.033
	Mean	-	-	0.033	0.007	0.009	0.009	0.019
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (0, 1)	4 (0, 4)	4 (0, 4)	4 (0, 4)	2 (0, 2)
B	Range	-	-	0.033 - 0.033	0.011 - 0.739	0.011 - 0.025	0.025 - 0.06	0.03 - 0.033
	Mean	-	-	0.033	0.199	0.015	0.037	0.032
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (0, 1)	4 (2, 2)	4 (0, 4)	4 (3, 1)	2 (0, 2)
Ba	Range	-	-	0.053 - 0.053	0.036 - 0.058	0.005 - 0.084	0.027 - 0.084	0.035 - 0.045
	Mean	-	-	0.053	0.045	0.042	0.05	0.04
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (1, 0)	4 (4, 0)	4 (3, 1)	4 (4, 0)	2 (2, 0)
Be	Range	-	-	-	0.01 - 0.011	0.001 - 0.011	0.001 - 0.011	-
	Mean	-	-	-	0.01	0.008	0.008	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	2 (0, 2)	4 (0, 4)	4 (0, 4)	0 (0, 0)
Ca	Range	-	-	8.65 - 8.65	8.535 - 11.83	7.15 - 11.514	20.21 - 38.011	8.31 - 8.31
	Mean	-	-	8.65	10.286	9.235	29.43	8.31
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (1, 0)	4 (4, 0)	4 (4, 0)	4 (4, 0)	1 (1, 0)
Cd	Range	-	-	0.033 - 0.033	0.001 - 0.011	0.001 - 0.011	0.001 - 0.011	0.004 - 0.033
	Mean	-	-	0.033	0.006	0.007	0.007	0.019
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (0, 1)	5 (0, 5)	5 (0, 5)	5 (0, 5)	2 (0, 2)
Cl-	Range	-	-	9.6 - 9.6	3.9 - 16.5	3 - 12.77	3 - 95	10.8 - 13.8
	Mean	-	-	9.6	7.472	6.791	57.221	12.3
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (1, 0)	6 (6, 0)	7 (6, 1)	7 (6, 1)	2 (2, 0)
Co	Range	-	-	-	0.002 - 0.011	0.002 - 0.011	0.002 - 0.011	0.004 - 0.004
	Mean	-	-	-	0.007	0.007	0.007	0.004
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	4 (0, 4)	5 (0, 5)	5 (0, 5)	1 (0, 1)
Cr6+	Range	-	-	-	0.02 - 0.1	0.02 - 0.1	0.02 - 0.1	-
	Mean	-	-	-	0.058	0.068	0.068	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	5 (0, 5)	5 (0, 5)	5 (0, 5)	0 (0, 0)
CrTotal	Range	-	-	0.033 - 0.033	0.002 - 0.011	0.01 - 0.011	0.01 - 0.011	0.01 - 0.033
	Mean	-	-	0.033	0.008	0.011	0.011	0.022
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (0, 1)	4 (1, 3)	3 (0, 3)	3 (0, 3)	2 (0, 2)

	Range	-	-	0.039 - 0.039	0.011 - 1	0.01 - 0.011	0.01 - 0.013	0.027 - 0.063
Cu	Mean	-	-	0.039	0.262	0.011	0.011	0.045
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (1, 0)	4 (0, 4)	4 (0, 4)	4 (1, 3)	2 (1, 1)
	Range	-	-	0.5 - 0.5	0.02 - 0.03	0.02 - 0.03	0.02 - 0.03	0.5 - 0.5
CN-	Mean	-	-	0.5	0.025	0.028	0.028	0.5
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (0, 1)	2 (0, 2)	4 (0, 4)	4 (0, 4)	1 (0, 1)
	Range	-	-	1.47 - 1.47	1.11 - 2.4	0.3 - 2.315	0.3 - 1.71	0.881 - 1.06
Fe	Mean	-	-	1.47	1.562	0.955	1.158	0.971
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (1, 0)	5 (5, 0)	6 (5, 1)	6 (5, 1)	2 (2, 0)
Hg	Range	-	-	0.033 - 0.033	0.003 - 0.022	0.003 - 0.011	0.003 - 0.011	0.022 - 0.033
	Mean	-	-	0.033	0.011	0.008	0.007	0.028
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (0, 1)	4 (0, 4)	5 (0, 5)	4 (0, 4)	2 (0, 2)
	Range	-	-	1.8 - 1.8	1.4 - 1.4	-	-	1.77 - 1.98
K	Mean	-	-	1.8	1.4	-	-	1.875
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (0, 1)	1 (1, 0)	0 (0, 0)	0 (0, 0)	2 (2, 0)
	Range	-	-	0.003 - 0.003	0.004 - 0.011	0.011 - 0.011	0.011 - 0.011	0.004 - 0.022
Li	Mean	-	-	0.003	0.009	0.011	0.011	0.013
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (0, 1)	3 (0, 3)	3 (0, 3)	3 (0, 3)	2 (1, 1)
	Range	-	-	3.08 - 3.08	0.7 - 4.237	0.1 - 3.275	2.62 - 6.395	0.5 - 2.63
Mg	Mean	-	-	3.08	3.143	2.017	4.736	1.565
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (1, 0)	5 (5, 0)	6 (6, 0)	6 (6, 0)	2 (2, 0)
	Range	-	-	0.063 - 0.063	0.033 - 0.16	0.037 - 0.098	0.053 - 0.187	0.045 - 0.049
Mn	Mean	-	-	0.063	0.101	0.058	0.095	0.047
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (1, 0)	5 (5, 0)	4 (4, 0)	4 (4, 0)	2 (2, 0)
	Range	-	-	-	0.001 - 0.011	0.011 - 0.011	0.011 - 0.011	-
Mo	Mean	-	-	-	0.008	0.011	0.011	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	3 (0, 3)	3 (0, 3)	3 (0, 3)	0 (0, 0)
	Range	-	-	-	5.03 - 8.96	0.96 - 8.18	3.55 - 129	3.56 - 6.94
Na	Mean	-	-	-	6.967	4.878	56.927	5.25
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	5 (5, 0)	4 (4, 0)	4 (4, 0)	2 (2, 0)
	Range	-	-	0.006 - 0.006	0.003 - 0.013	0.003 - 0.011	0.005 - 0.011	0.005 - 0.033
Ni	Mean	-	-	0.006	0.008	0.009	0.009	0.019
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (1, 0)	5 (3, 2)	4 (0, 4)	3 (1, 2)	2 (1, 1)
	Range	-	-	0.033 - 0.033	0.01 - 0.021	0.01 - 0.011	0.01 - 0.011	0.009 - 0.033
Pb	Mean	-	-	0.033	0.013	0.011	0.011	0.021
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (0, 1)	4 (2, 2)	5 (0, 5)	5 (0, 5)	2 (1, 1)
	Range	-	-	-	0.01 - 0.448	0.01 - 0.2	0.01 - 0.242	0.02 - 0.02
Phenol	Mean	-	-	-	0.17	0.104	0.112	0.02
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	4 (1, 3)	5 (0, 5)	5 (1, 4)	1 (0, 1)
	Range	1.8 - 1.8	-	0.5 - 0.8	0.9 - 2	2 - 9.6	2 - 8.7	1 - 1.2
S2-	Mean	1.8	-	0.65	1.633	5.4	5.25	1.1
	N (A, B)	1 (1, 0)	0 (0, 0)	2 (1, 1)	3 (1, 2)	4 (3, 1)	4 (3, 1)	2 (2, 0)
	Range	-	-	2.7 - 2.7	2.1 - 28.3	8.3 - 33.9	8 - 138	2.1 - 2.5
SO42-	Mean	-	-	2.7	17.842	14.517	77.321	2.3
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (1, 0)	6 (6, 0)	7 (7, 0)	7 (7, 0)	2 (2, 0)
	Range	-	-	-	-	-	-	-
Sb	Mean	-	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
	Range	-	-	0.033 - 0.033	0.005 - 0.011	0.005 - 0.011	0.005 - 0.011	0.011 - 0.033
Se	Mean	-	-	0.033	0.01	0.009	0.009	0.022
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (0, 1)	4 (0, 4)	5 (0, 5)	5 (0, 5)	2 (0, 2)
Va	Range	-	-	-	0.011 - 0.011	0.002 - 0.011	0.007 - 0.011	-

	Mean	-	-	-	0.011	0.009	0.01	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	2 (0, 2)	4 (0, 4)	4 (1, 3)	0 (0, 0)
	Range	-	-	0.033 - 0.033	0.009 - 0.043	0.011 - 0.044	0.022 - 0.198	0.008 - 0.033
Zn	Mean	-	-	0.033	0.027	0.032	0.122	0.021
	N (A, B)	0 (0, 0)	0 (0, 0)	1 (0, 1)	4 (3, 1)	3 (2, 1)	3 (3, 0)	2 (0, 2)

* N: Number of records; A & B: Number of records above and below detection limits.

Table S2.2. Univariate statistics for toxic determinands in sub-basins S4 and S5.

Toxicant (mg/L)	Statistic	S4:1	S4:2	S4:3	S4:4	S4:5	S5:1
	Range	0.002 - 0.002	0.011 - 0.011	0.011 - 0.011	0.011 - 0.011	0.011 - 0.011	0.002 - 0.002
Ag	Mean	0.002	0.011	0.011	0.011	0.011	0.002
	N (A, B) *	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)
	Range	0.121 - 0.121	0.568 - 0.568	0.276 - 0.276	1.211 - 1.211	7.073 - 7.073	11.8 - 11.8
Al	Mean	0.121	0.568	0.276	1.211	7.073	11.8
	N (A, B)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)
	Range	0.003 - 0.003	0.013 - 0.013	0.016 - 0.016	0.02 - 0.02	0.011 - 0.011	-
As	Mean	0.003	0.013	0.016	0.02	0.011	-
	N (A, B)	1 (0, 1)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (0, 1)	0 (0, 0)
	Range	0.051 - 0.051	0.025 - 0.025	0.011 - 0.011	0.011 - 0.011	0.2 - 0.2	0.03 - 0.03
B	Mean	0.051	0.025	0.011	0.011	0.2	0.03
	N (A, B)	1 (1, 0)	1 (1, 0)	1 (0, 1)	1 (0, 1)	1 (1, 0)	1 (0, 1)
	Range	0.082 - 0.082	0.056 - 0.056	0.053 - 0.053	0.059 - 0.059	0.02 - 0.02	0.202 - 0.202
Ba	Mean	0.082	0.056	0.053	0.059	0.02	0.202
	N (A, B)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)
	Range	0.001 - 0.001	0.011 - 0.011	0.01 - 0.01	0.01 - 0.01	0.011 - 0.011	-
Be	Mean	0.001	0.011	0.01	0.01	0.011	-
	N (A, B)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	0 (0, 0)
	Range	14.4 - 14.4	-	3.721 - 3.721	3.762 - 3.762	-	-
Ca	Mean	14.4	-	3.721	3.762	-	-
	N (A, B)	1 (1, 0)	0 (0, 0)	1 (1, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)
	Range	-	0.011 - 0.011	0.01 - 0.01	0.01 - 0.01	0.011 - 0.011	-
Cd	Mean	-	0.011	0.01	0.01	0.011	-
	N (A, B)	0 (0, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	0 (0, 0)
	Range	4.17 - 4.17	27.5 - 27.5	12.88 - 12.88	11.67 - 11.67	3 - 3	23.5 - 23.5
Cl-	Mean	4.17	27.5	12.88	11.67	3	23.5
	N (A, B)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (0, 1)	1 (1, 0)
	Range	0.002 - 0.002	0.011 - 0.011	-	-	0.011 - 0.011	-
Co	Mean	0.002	0.011	-	-	0.011	-
	N (A, B)	1 (0, 1)	1 (0, 1)	0 (0, 0)	0 (0, 0)	1 (0, 1)	0 (0, 0)
	Range	-	-	-	-	-	-
Cr6+	Mean	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
	Range	0.002 - 0.002	0.011 - 0.011	0.01 - 0.01	0.01 - 0.01	0.041 - 0.041	0.01 - 0.01
CrTotal	Mean	0.002	0.011	0.01	0.01	0.041	0.01
	N (A, B)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (1, 0)	1 (0, 1)
	Range	0.01 - 0.01	0.011 - 0.011	0.011 - 0.011	0.011 - 0.011	0.021 - 0.021	0.02 - 0.02
Cu	Mean	0.01	0.011	0.011	0.011	0.021	0.02
	N (A, B)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (1, 0)	1 (1, 0)
	Range	0.03 - 0.03	0.02 - 0.02	0.03 - 0.03	0.03 - 0.03	0.02 - 0.02	0.5 - 0.5
CN-	Mean	0.03	0.02	0.03	0.03	0.02	0.5
	N (A, B)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)
Fe	Range	0.3 - 0.3	4.12 - 4.12	-	-	78.763 - 78.763	13.7 - 13.7

	Mean	0.3	4.12	-	-	78.763	13.7
	N (A, B)	1 (0, 1)	1 (1, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)	1 (1, 0)
Hg	Range	0.003 - 0.003	0.011 - 0.011	0.01 - 0.01	0.01 - 0.01	0.011 - 0.011	0.022 - 0.022
	Mean	0.003	0.011	0.01	0.01	0.011	0.022
	N (A, B)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)
	Range	2.02 - 2.02	-	-	-	-	5.84 - 5.84
K	Mean	2.02	-	-	-	-	5.84
	N (A, B)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)
	Range	0.011 - 0.011	0.038 - 0.038	-	-	0.287 - 0.287	-
Li	Mean	0.011	0.038	-	-	0.287	-
	N (A, B)	1 (1, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)
	Range	12.83 - 12.83	-	-	-	-	10.8 - 10.8
Mg	Mean	12.83	-	-	-	-	10.8
	N (A, B)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)
	Range	0.25 - 0.25	2.149 - 2.149	0.047 - 0.047	0.059 - 0.059	4.964 - 4.964	0.154 - 0.154
Mn	Mean	0.25	2.149	0.047	0.059	4.964	0.154
	N (A, B)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)
	Range	0.001 - 0.001	0.011 - 0.011	0.011 - 0.011	0.011 - 0.011	0.011 - 0.011	-
Mo	Mean	0.001	0.011	0.011	0.011	0.011	-
	N (A, B)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	0 (0, 0)
	Range	1.31 - 1.31	-	-	-	-	32.4 - 32.4
Na	Mean	1.31	-	-	-	-	32.4
	N (A, B)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (1, 0)
	Range	0.004 - 0.004	0.117 - 0.117	0.011 - 0.011	0.011 - 0.011	0.034 - 0.034	0.019 - 0.019
Ni	Mean	0.004	0.117	0.011	0.011	0.034	0.019
	N (A, B)	1 (1, 0)	1 (1, 0)	1 (0, 1)	1 (0, 1)	1 (1, 0)	1 (1, 0)
	Range	0.01 - 0.01	0.061 - 0.061	0.011 - 0.011	0.011 - 0.011	0.023 - 0.023	0.022 - 0.022
Pb	Mean	0.01	0.061	0.011	0.011	0.023	0.022
	N (A, B)	1 (0, 1)	1 (1, 0)	1 (0, 1)	1 (0, 1)	1 (1, 0)	1 (1, 0)
	Range	0.1 - 0.1	0.2 - 0.2	0.2 - 0.2	0.2 - 0.2	0.2 - 0.2	0.02 - 0.02
Phenol	Mean	0.1	0.2	0.2	0.2	0.2	0.02
	N (A, B)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)
	Range	2 - 2	2 - 2	2 - 2	2 - 2	27.7 - 27.7	0.5 - 0.5
S2-	Mean	2	2	2	2	27.7	0.5
	N (A, B)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (1, 0)	1 (0, 1)
	Range	50.2 - 50.2	360 - 360	0.5 - 0.5	145 - 145	2430 - 2430	14.6 - 14.6
SO42-	Mean	50.2	360	0.5	145	2430	14.6
	N (A, B)	1 (1, 0)	1 (1, 0)	1 (0, 1)	1 (1, 0)	1 (1, 0)	1 (1, 0)
	Range	0.002 - 0.002	-	-	-	-	-
Sb	Mean	0.002	-	-	-	-	-
	N (A, B)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
	Range	0.005 - 0.005	0.011 - 0.011	0.011 - 0.011	0.011 - 0.011	0.011 - 0.011	-
Se	Mean	0.005	0.011	0.011	0.011	0.011	-
	N (A, B)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	0 (0, 0)
	Range	0.002 - 0.002	0.011 - 0.011	-	-	0.011 - 0.011	-
Va	Mean	0.002	0.011	-	-	0.011	-
	N (A, B)	1 (0, 1)	1 (0, 1)	0 (0, 0)	0 (0, 0)	1 (0, 1)	0 (0, 0)
	Range	0.025 - 0.025	0.187 - 0.187	0.011 - 0.011	0.011 - 0.011	0.85 - 0.85	0.051 - 0.051
Zn	Mean	0.025	0.187	0.011	0.011	0.85	0.051
	N (A, B)	1 (0, 1)	1 (1, 0)	1 (0, 1)	1 (0, 1)	1 (1, 0)	1 (1, 0)

* N: Number of records; A & B: Number of records above and below detection limits.

Table S2.3. Univariate statistics for toxic determinands in sub-basin S2: Part 1.

Toxicant (mg/L)	Statistic	S2:1	S2:2	S2:3	S2:4	S2:5	S2:6
Ag	Range	0.033 - 0.048	0.033 - 0.033	-	-	-	0.002 - 0.033
	Mean	0.041	0.033	-	-	-	0.01
	N (A, B) *	2 (1, 1)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	7 (1, 6)
Al	Range	0.172 - 0.236	0.182 - 0.182	-	-	-	0.214 - 0.918
	Mean	0.204	0.182	-	-	-	0.512
	N (A, B)	2 (1, 1)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	6 (5, 1)
As	Range	0.005 - 0.033	0.033 - 0.033	-	-	-	0.003 - 0.033
	Mean	0.019	0.033	-	-	-	0.012
	N (A, B)	2 (0, 2)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	6 (0, 6)
B	Range	0.03 - 0.033	0.033 - 0.033	-	-	-	0.011 - 0.033
	Mean	0.032	0.033	-	-	-	0.02
	N (A, B)	2 (0, 2)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	6 (0, 6)
Ba	Range	0.041 - 0.075	0.076 - 0.076	-	-	-	0.03 - 0.069
	Mean	0.058	0.076	-	-	-	0.052
	N (A, B)	2 (2, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	6 (6, 0)
Be	Range	-	-	-	-	-	0.001 - 0.011
	Mean	-	-	-	-	-	0.008
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	4 (0, 4)
Ca	Range	4.84 - 4.84	4.62 - 4.62	-	-	-	6.879 - 9.319
	Mean	4.84	4.62	-	-	-	8.066
	N (A, B)	1 (1, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	5 (5, 0)
Cd	Range	0.004 - 0.033	0.033 - 0.033	-	-	-	0.001 - 0.033
	Mean	0.019	0.033	-	-	-	0.01
	N (A, B)	2 (0, 2)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	7 (0, 7)
Cl-	Range	11.7 - 12.1	9.8 - 9.8	-	-	-	2.5 - 10.3
	Mean	11.9	9.8	-	-	-	5.215
	N (A, B)	2 (2, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	8 (7, 1)
Co	Range	0.004 - 0.004	-	-	-	-	0.002 - 0.011
	Mean	0.004	-	-	-	-	0.007
	N (A, B)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	6 (1, 5)
Cr6+	Range	-	-	-	-	-	0.02 - 0.1
	Mean	-	-	-	-	-	0.068
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	5 (0, 5)
CrTotal	Range	0.01 - 0.033	0.033 - 0.033	-	-	-	0.01 - 0.033
	Mean	0.022	0.033	-	-	-	0.015
	N (A, B)	2 (0, 2)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	5 (0, 5)
Cu	Range	0.027 - 0.05	0.059 - 0.059	-	-	-	0.01 - 0.059
	Mean	0.039	0.059	-	-	-	0.021
	N (A, B)	2 (2, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	6 (1, 5)
CN-	Range	0.5 - 0.5	0.5 - 0.5	-	-	-	0.02 - 0.5
	Mean	0.5	0.5	-	-	-	0.145
	N (A, B)	1 (0, 1)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	4 (0, 4)
Fe	Range	0.254 - 0.519	0.338 - 0.338	-	-	-	0.3 - 1.72
	Mean	0.387	0.338	-	-	-	1.201
	N (A, B)	2 (2, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	8 (7, 1)
Hg	Range	0.026 - 0.033	0.033 - 0.033	-	-	-	0.003 - 0.033
	Mean	0.03	0.033	-	-	-	0.013
	N (A, B)	2 (1, 1)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	7 (0, 7)
K	Range	1.01 - 1.8	1.8 - 1.8	-	-	-	1.8 - 2.17
	Mean	1.405	1.8	-	-	-	1.985

	N (A, B)	2 (1, 1)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	2 (1, 1)
Li	Range	0.003 - 0.004	0.003 - 0.003	-	-	-	0.003 - 0.011
	Mean	0.004	0.003	-	-	-	0.008
	N (A, B)	2 (0, 2)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	5 (0, 5)
Mg	Range	0.24 - 1.04	1.01 - 1.01	-	-	-	1.8 - 3.5
	Mean	0.64	1.01	-	-	-	2.804
	N (A, B)	2 (1, 1)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	8 (8, 0)
Mn	Range	0.03 - 0.051	0.037 - 0.037	-	-	-	0.092 - 0.182
	Mean	0.041	0.037	-	-	-	0.144
	N (A, B)	2 (2, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	6 (6, 0)
Mo	Range	-	-	-	-	-	0.011 - 0.011
	Mean	-	-	-	-	-	0.011
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	3 (0, 3)
Na	Range	3.23 - 3.56	2.2 - 2.2	6.07 - 6.07	-	-	0.643 - 6.99
	Mean	3.395	2.2	6.07	-	-	4.53
	N (A, B)	2 (1, 1)	1 (1, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	6 (6, 0)
Ni	Range	0.003 - 0.033	0.033 - 0.033	-	-	-	0.007 - 0.023
	Mean	0.018	0.033	-	-	-	0.012
	N (A, B)	2 (0, 2)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	6 (4, 2)
Pb	Range	0.012 - 0.033	0.033 - 0.033	-	-	-	0.01 - 0.033
	Mean	0.023	0.033	-	-	-	0.017
	N (A, B)	2 (1, 1)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	7 (3, 4)
Phenol	Range	0.02 - 0.02	-	-	-	-	0.01 - 0.2
	Mean	0.02	-	-	-	-	0.088
	N (A, B)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	5 (0, 5)
S2-	Range	0.7 - 1.4	0.5 - 0.5	0.5 - 0.5	0.5 - 0.5	0.5 - 0.5	0.73 - 2.1
	Mean	1.05	0.5	0.5	0.5	0.5	1.505
	N (A, B)	2 (2, 0)	1 (1, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)	6 (4, 2)
SO42-	Range	2 - 2.5	2.5 - 2.5	-	-	-	18 - 44.5
	Mean	2.25	2.5	-	-	-	26.694
	N (A, B)	2 (2, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	8 (8, 0)
Sb	Range	-	-	-	-	-	-
	Mean	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
Se	Range	0.011 - 0.033	0.033 - 0.033	-	-	-	0.005 - 0.033
	Mean	0.022	0.033	-	-	-	0.012
	N (A, B)	2 (0, 2)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	7 (0, 7)
Va	Range	-	-	-	-	-	0.002 - 0.011
	Mean	-	-	-	-	-	0.009
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	4 (0, 4)
Zn	Range	0.012 - 0.054	0.046 - 0.046	-	-	-	0.011 - 0.093
	Mean	0.033	0.046	-	-	-	0.038
	N (A, B)	2 (2, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	5 (3, 2)

* N: Number of records; A & B: Number of records above and below detection limits.

Table S2.4. Univariate statistics for toxic determinands in sub-basin S2: Part 2.

Toxicant (mg/L)	Statistic	S2:7	S2:8	S2:9	S2:10	S2:11	S2:12	S2:13
Ag	Range	0.011 - 0.011	-	0.011 - 0.011	-	0.011 - 0.011	0.011 - 0.011	0.011 - 0.011
	Mean	0.011	-	0.011	-	0.011	0.011	0.011
	N (A, B) *	1 (0, 1)	0 (0, 0)	1 (0, 1)	0 (0, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)
Al	Range	1.076 - 1.076	-	21.991 - 21.991	-	0.325 - 0.325	0.116 - 0.116	0.447 - 0.447
	Mean	1.076	-	21.991	-	0.325	0.116	0.447

	N (A, B)	1 (1, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)
	Range	0.011 - 0.011	-	0.022 - 0.022	-	0.018 - 0.018	0.01 - 0.01	0.01 - 0.01
As	Mean	0.011	-	0.022	-	0.018	0.01	0.01
	N (A, B)	1 (0, 1)	0 (0, 0)	1 (1, 0)	0 (0, 0)	1 (1, 0)	1 (0, 1)	1 (0, 1)
	Range	0.021 - 0.021	-	0.403 - 0.403	-	-	-	-
B	Mean	0.021	-	0.403	-	-	-	-
	N (A, B)	1 (1, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
	Range	0.077 - 0.077	-	0.068 - 0.068	-	0.057 - 0.057	0.054 - 0.054	0.054 - 0.054
Ba	Mean	0.077	-	0.068	-	0.057	0.054	0.054
	N (A, B)	1 (1, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)
	Range	0.011 - 0.011	-	0.011 - 0.011	-	-	-	-
Be	Mean	0.011	-	0.011	-	-	-	-
	N (A, B)	1 (0, 1)	0 (0, 0)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
	Range	-	-	-	-	-	-	-
Ca	Mean	-	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
	Range	0.011 - 0.011	-	0.011 - 0.011	-	0.011 - 0.011	0.011 - 0.011	0.011 - 0.011
Cd	Mean	0.011	-	0.011	-	0.011	0.011	0.011
	N (A, B)	1 (0, 1)	0 (0, 0)	1 (0, 1)	0 (0, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)
	Range	3.29 - 3.29	3 - 3	2.54 - 3	3 - 3	4.27 - 4.27	3.85 - 3.85	4.37 - 4.37
Cl-	Mean	3.29	3	2.77	3	4.27	3.85	4.37
	N (A, B)	1 (1, 0)	1 (0, 1)	2 (1, 1)	1 (0, 1)	1 (1, 0)	1 (1, 0)	1 (1, 0)
	Range	0.011 - 0.011	-	0.246 - 0.246	-	-	-	-
Co	Mean	0.011	-	0.246	-	-	-	-
	N (A, B)	1 (0, 1)	0 (0, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
	Range	-	-	-	-	-	-	-
Cr6+	Mean	-	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
	Range	0.011 - 0.011	-	0.136 - 0.136	-	0.01 - 0.01	0.01 - 0.01	0.01 - 0.01
CrTotal	Mean	0.011	-	0.136	-	0.01	0.01	0.01
	N (A, B)	1 (0, 1)	0 (0, 0)	1 (1, 0)	0 (0, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)
	Range	0.016 - 0.016	-	0.242 - 0.242	-	0.011 - 0.011	0.011 - 0.011	0.011 - 0.011
Cu	Mean	0.016	-	0.242	-	0.011	0.011	0.011
	N (A, B)	1 (1, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)
	Range	-	-	-	-	0.03 - 0.03	0.03 - 0.03	0.03 - 0.03
CN-	Mean	-	-	-	-	0.03	0.03	0.03
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)
	Range	9.1 - 9.1	-	187 - 187	-	1.224 - 1.224	0.862 - 0.862	1.971 - 1.971
Fe	Mean	9.1	-	187	-	1.224	0.862	1.971
	N (A, B)	1 (1, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)
Hg	Range	0.011 - 0.011	-	0.011 - 0.011	-	0.01 - 0.01	0.01 - 0.01	0.01 - 0.01
	Mean	0.011	-	0.011	-	0.01	0.01	0.01
	N (A, B)	1 (0, 1)	0 (0, 0)	1 (0, 1)	0 (0, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)
	Range	-	-	-	-	-	-	-
K	Mean	-	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
	Range	0.043 - 0.043	-	0.156 - 0.156	-	-	-	-
Li	Mean	0.043	-	0.156	-	-	-	-
	N (A, B)	1 (1, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
	Range	-	-	-	-	-	-	-
Mg	Mean	-	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)

	Range	0.787 - 0.787	-	3.948 - 3.948	-	-	-	-
Mn	Mean	0.787	-	3.948	-	-	-	-
	N (A, B)	1 (1, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
	Range	0.011 - 0.011	-	0.011 - 0.011	-	-	-	-
Mo	Mean	0.011	-	0.011	-	-	-	-
	N (A, B)	1 (0, 1)	0 (0, 0)	1 (0, 1)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
	Range	-	-	-	-	-	-	-
Na	Mean	-	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
	Range	0.147 - 0.147	-	0.559 - 0.559	-	0.011 - 0.011	0.011 - 0.011	0.011 - 0.011
Ni	Mean	0.147	-	0.559	-	0.011	0.011	0.011
	N (A, B)	1 (1, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)
	Range	0.011 - 0.011	-	0.061 - 0.061	-	0.011 - 0.011	0.011 - 0.011	0.011 - 0.011
Pb	Mean	0.011	-	0.061	-	0.011	0.011	0.011
	N (A, B)	1 (0, 1)	0 (0, 0)	1 (1, 0)	0 (0, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)
	Range	0.2 - 0.2	0.01 - 0.01	0.01 - 0.27	0.01 - 0.01	0.2 - 0.2	0.2 - 0.2	0.2 - 0.2
Phenol	Mean	0.2	0.01	0.14	0.01	0.2	0.2	0.2
	N (A, B)	1 (0, 1)	1 (0, 1)	2 (1, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)	1 (0, 1)
	Range	10.2 - 10.2	2 - 2	12.6 - 36.4	2.8 - 2.8	2 - 2	2 - 2	2 - 2
S2-	Mean	10.2	2	24.5	2.8	2	2	2
	N (A, B)	1 (1, 0)	1 (0, 1)	2 (2, 0)	1 (1, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)
	Range	92.35 - 92.35	86 - 86	658 - 801	547 - 547	10.37 - 10.37	4.25 - 4.25	25.87 - 25.87
SO42-	Mean	92.35	86	729.5	547	10.37	4.25	25.87
	N (A, B)	1 (1, 0)	1 (1, 0)	2 (2, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)	1 (1, 0)
	Range	-	-	-	-	-	-	-
Sb	Mean	-	-	-	-	-	-	-
	N (A, B)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
	Range	0.011 - 0.011	-	0.011 - 0.011	-	0.011 - 0.011	0.011 - 0.011	0.011 - 0.011
Se	Mean	0.011	-	0.011	-	0.011	0.011	0.011
	N (A, B)	1 (0, 1)	0 (0, 0)	1 (0, 1)	0 (0, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)
	Range	0.011 - 0.011	-	0.034 - 0.034	-	-	-	-
Va	Mean	0.011	-	0.034	-	-	-	-
	N (A, B)	1 (0, 1)	0 (0, 0)	1 (1, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)	0 (0, 0)
	Range	0.452 - 0.452	-	1.981 - 1.981	-	0.011 - 0.011	0.011 - 0.011	0.011 - 0.011
Zn	Mean	0.452	-	1.981	-	0.011	0.011	0.011
	N (A, B)	1 (1, 0)	0 (0, 0)	1 (1, 0)	0 (0, 0)	1 (0, 1)	1 (0, 1)	1 (0, 1)

* N: Number of records; A & B: Number of records above and below detection limits.

S3. Spatiotemporal distribution of water quality

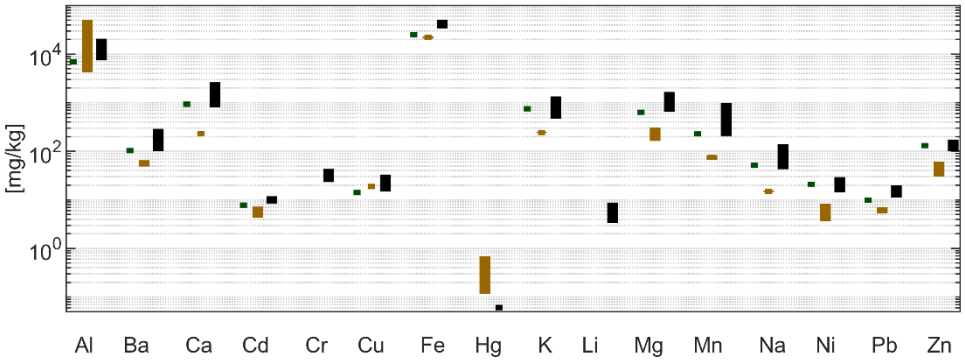

Figure S3.1. Spatial distribution of metals in sediments (green Cluster 3, yellor c4, black c6.

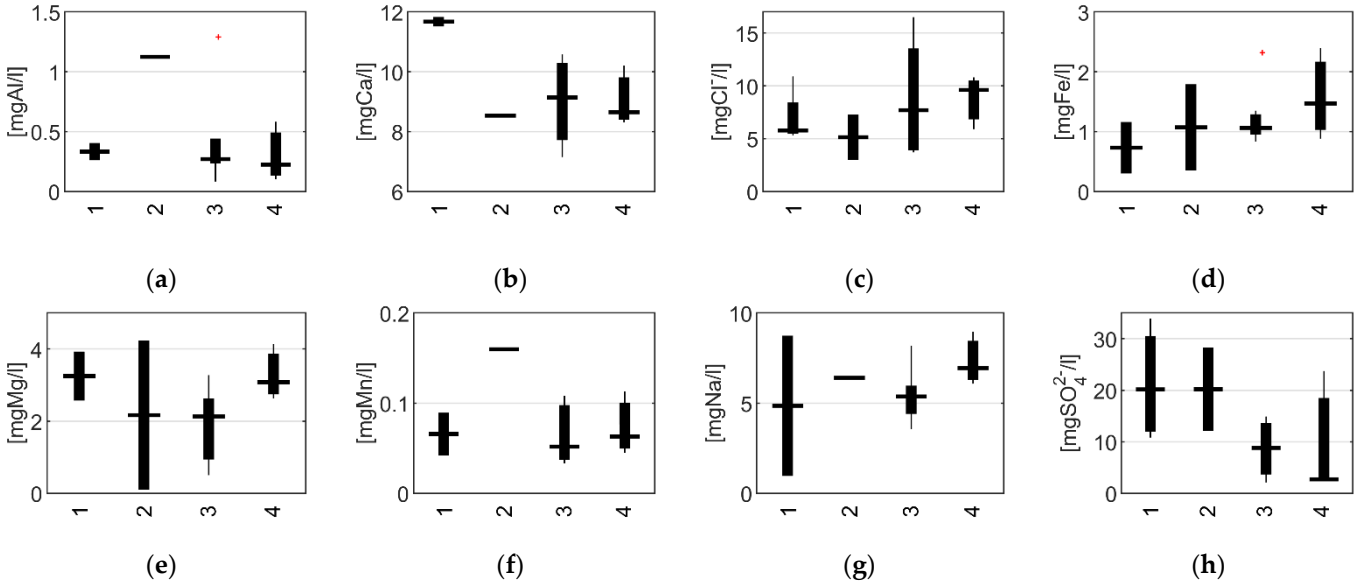

Figure S3.2. Temporal distribution of toxicants in C6: (**a**) Al; (**b**) Ca; (**c**) Cl^-; (**d**) Fe; (**e**) Mg; (**f**) Mn; (**g**) Na; (**h**) SO_4^{2-}.

S4. Characterization of river hydraulics and solute transport

Table S4.1. Geomorphology of all modeling segments.

Stream (# of segments)	Segments	Slope (S) [m/m]	Drainage Area (A) [km²]	$SA^{0.4}$	Geomorphology class
A (221 segments)	1-4	0.045	12.15	0.123	Step-pool
	5-7	0.082	12.43	0.223	Cascade
	8-18	0.041	13.33	0.116	Step-pool
	19-21	0.087	13.57	0.247	Cascade
	22-25	0.052	13.61	0.148	Step-pool
	26-28	0.075	13.68	0.214	Cascade
	29-33	0.044	13.82	0.125	Step-pool
	34-39	0.077	13.93	0.222	Cascade
	40-43	0.051	14.26	0.146	Step-pool
	44-62	0.115	15.43	0.344	Cascade
	63-71	0.054	15.94	0.164	Step-pool

Stream (# of segments)	Segments	Slope (S) [m/m]	Drainage Area (A) [km²]	$SA^{0.4}$	Geomorphology class
	72-74	0.069	16.01	0.210	Cascade
	75-84	0.025	16.18	0.076	Plane Bed
	85-90	0.041	17.17	0.129	Step-pool
	91-108	0.013	17.72	0.041	Pool-riffle
	109-118	0.043	18.11	0.137	Step-pool
	119-126	0.088	18.63	0.283	Cascade
	127-130	0.060	19.28	0.196	Step-pool
	131-142	0.084	19.76	0.278	Cascade
	143-151	0.048	20.07	0.158	Step-pool
	152-166	0.101	21.03	0.340	Cascade
	167-178	0.037	22.31	0.130	Step-pool
	179-181	0.095	22.63	0.331	Cascade
	182-187	0.037	22.82	0.130	Step-pool
	188-221	0.006	49.80	0.028	Pool-riffle
B (99 segments)	1-22	0.002	170.23	0.018	Pool-riffle
	23-44	0.002	172.34	0.018	Pool-riffle
	45-66	0.002	175.49	0.018	Pool-riffle
	67-89	0.002	178.01	0.018	Pool-riffle
	90-99	0.002	179.99	0.014	Pool-riffle
C (90 segments)	1-22	0.002	252.40	0.013	Pool-riffle
	23-47	0.002	258.88	0.018	Pool-riffle
	48-83	0.001	281.32	0.007	Pool-riffle
	84-90	0.001	290.07	0.007	Pool-riffle

Table S4.2. Hydraulic features of all modeled streams and segments.

Stream (# of segments)	Segments	Mean Length [m]	Mean Slope [m/m]	Mean Width [m]	n-Manning (Eq. 4)	a, b, α, β (Eq. 3)	Q [m³/s]	A [m²]	D [m²/s] (Eq. 6)
A (221 segments)	1-188	42.5	0.06	2.5	0.080	-	0.05	0.87	0.10
	189-196	43.6	7.41 E-3	2.5	0.080	-	0.05	0.87	0.33
	197-210	48.5	7.41 E-3	2.7	0.060	-	0.01	0.38	0.33
	211-213	78.8	7.41 E-3	2.7	0.060	-	0.01	0.38	0.33
	214-221	66.3	1.45 E-3	2.7	0.060	-	0.01	0.38	0.33
B (99 segments)	1-99	49.4	1.78 E-3	3.5	0.026	-	0.24	0.53	6.00
C (90 segments)	1-22	114.2	1.90 E-3	3.6	0.040	-	0.17	0.58	2.75
	23-47	98.8	1.90 E-3	4.0	0.040	-	0.18	0.61	2.75
	48-83	187.1	7.07 E-4	4.0	0.040	-	0.18	0.84	2.75
	84-90	129.7	-	-	-	0.55, 0.34, 0.32, 0.32	0.18	1.00	1.00

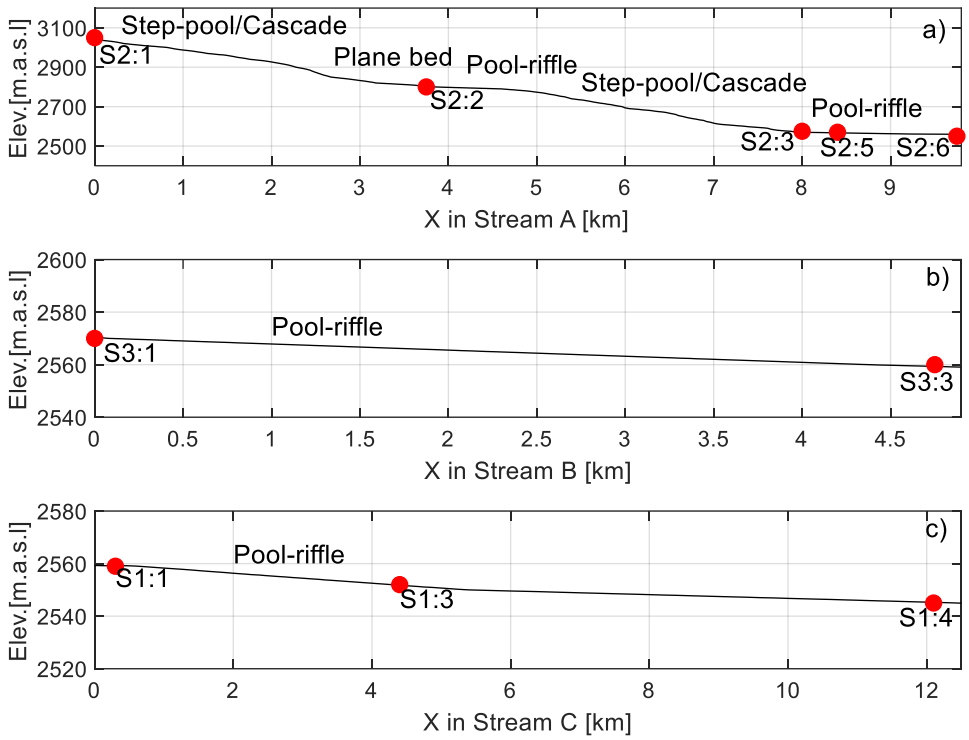

Figure S4.1 Longitudinal profile, geomorphology and monitoring sites: (**a**) Stream A; (**b**) Stream B; (**c**) Stream C.

S5. Model calibration plots

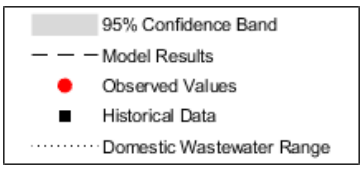

Figure S5.1. Legend.

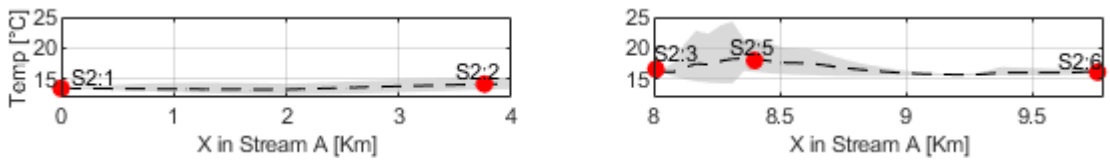

Figure S5.2. Calibration of temperature – Stream A.

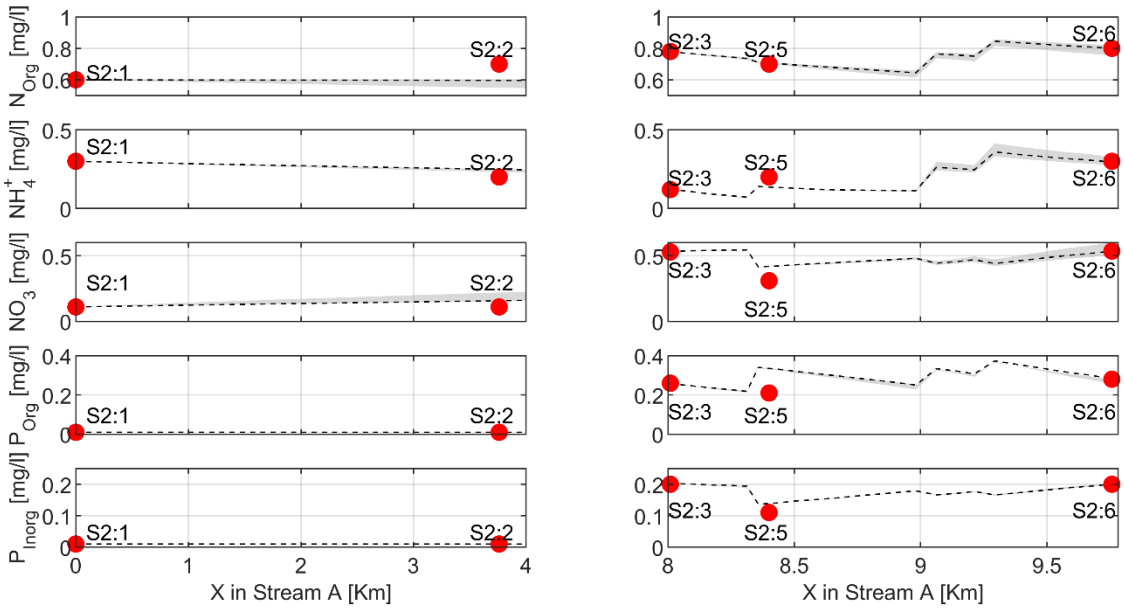

Figure S5.3. Calibration of Nutrients – Stream A.

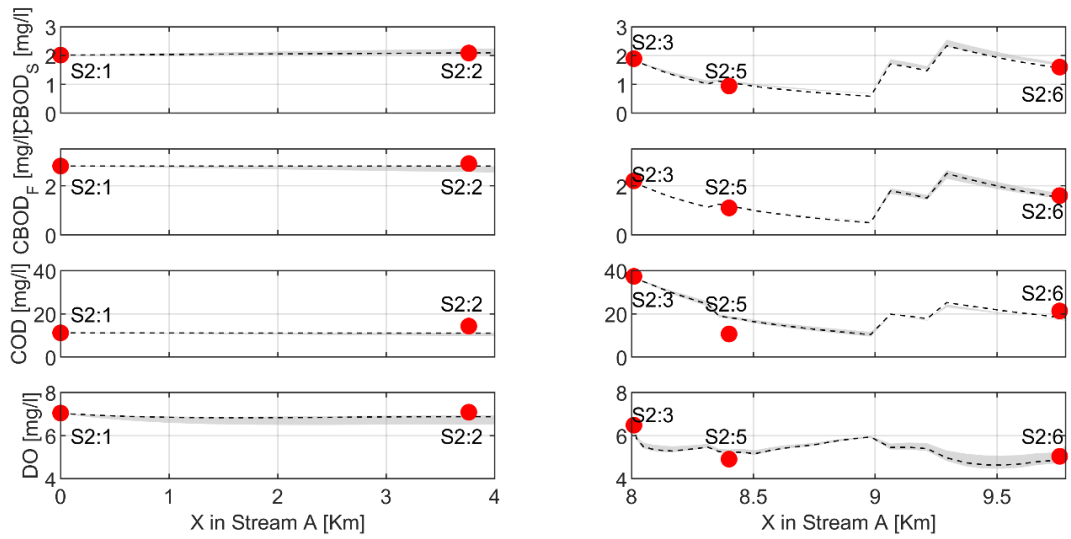

Figure S5.4. Calibration of dissolved oxygen and its demanding constituents – Stream A.

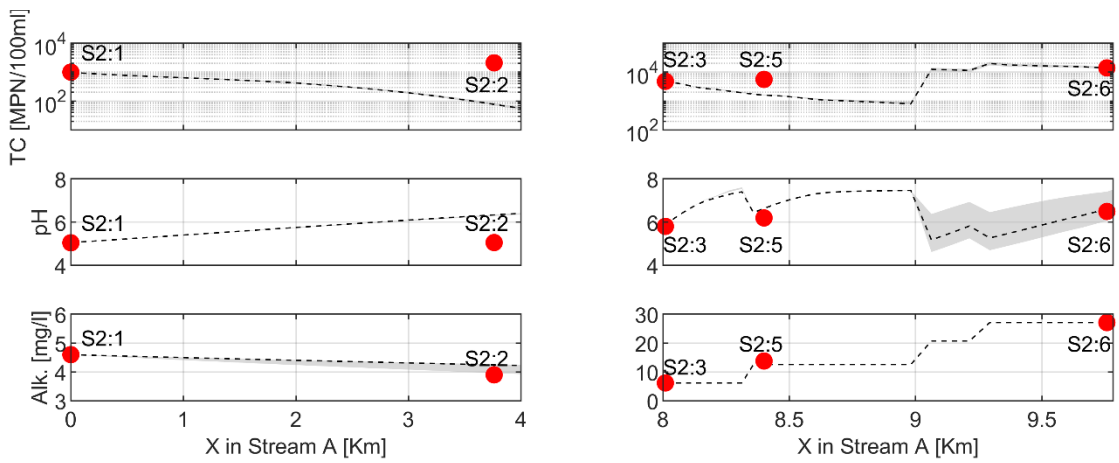

Figure S5.5. Calibration of pathogens, pH and alkalinity – Stream A.

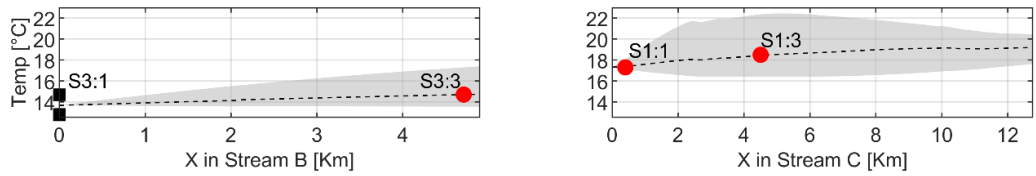

Figure S5.6. Calibration of temperature – Streams B and C.

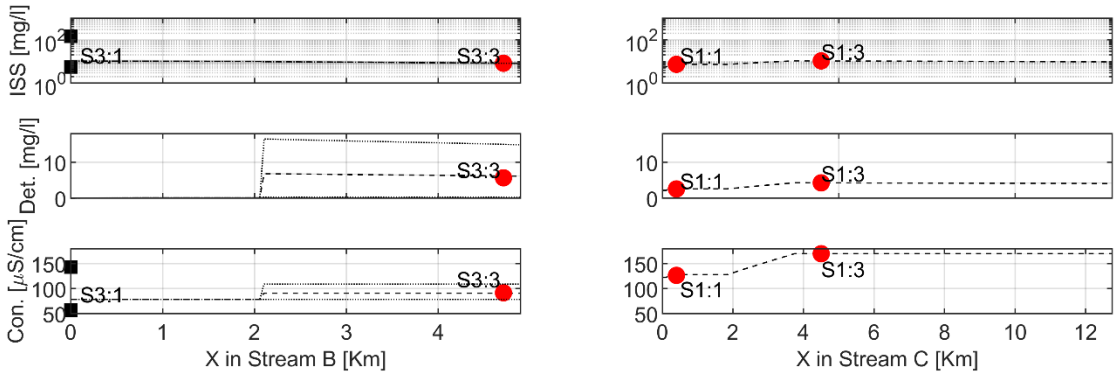

Figure S5.7. Calibration of solids and conductivity – Streams B and C.

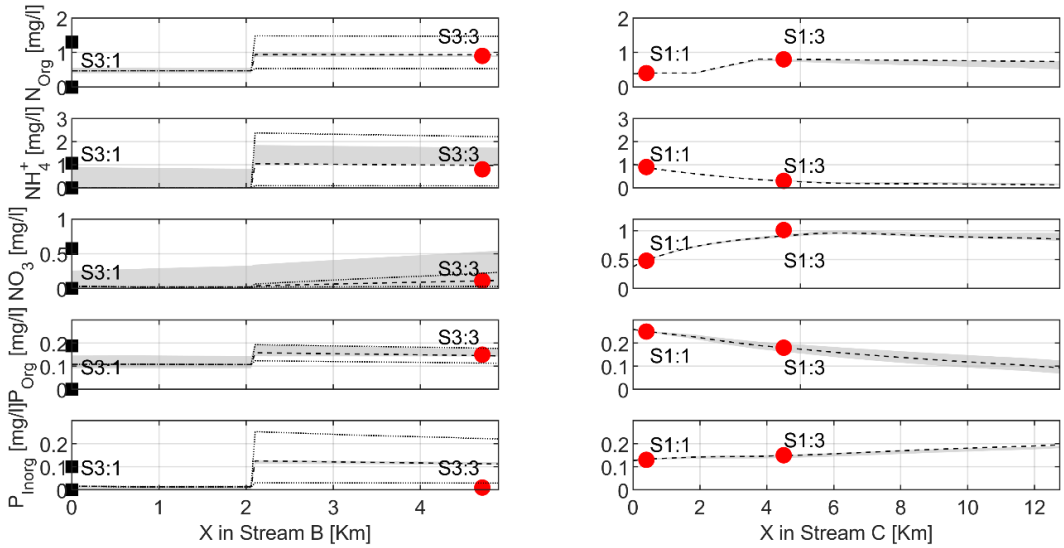

Figure S5.8. Calibration of nutrients – Streams B and C.

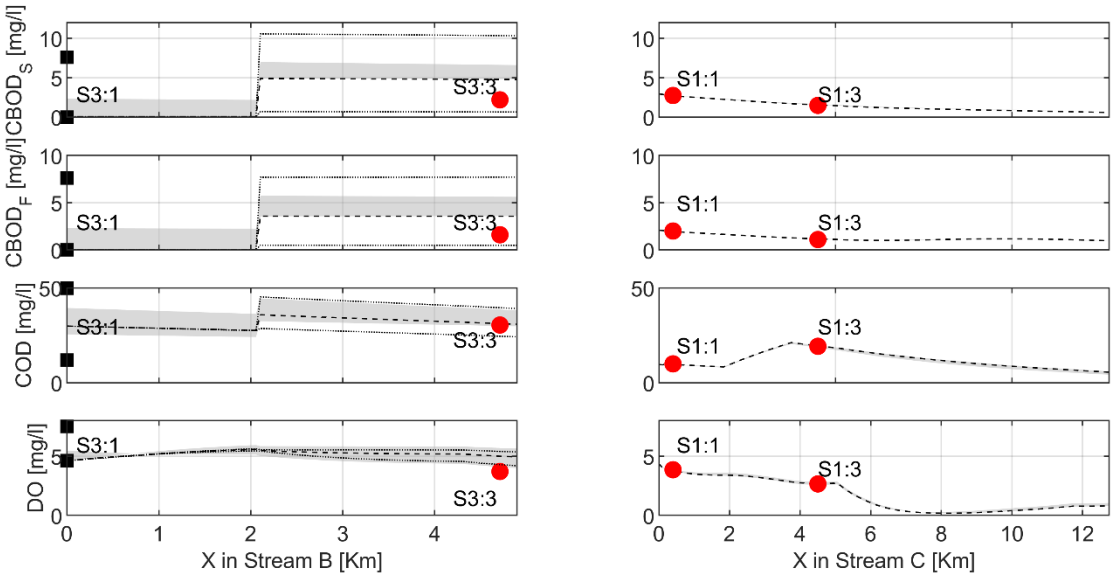

Figure S5.9. Calibration of dissolved oxygen and its demanding constituents – Streams B and C.

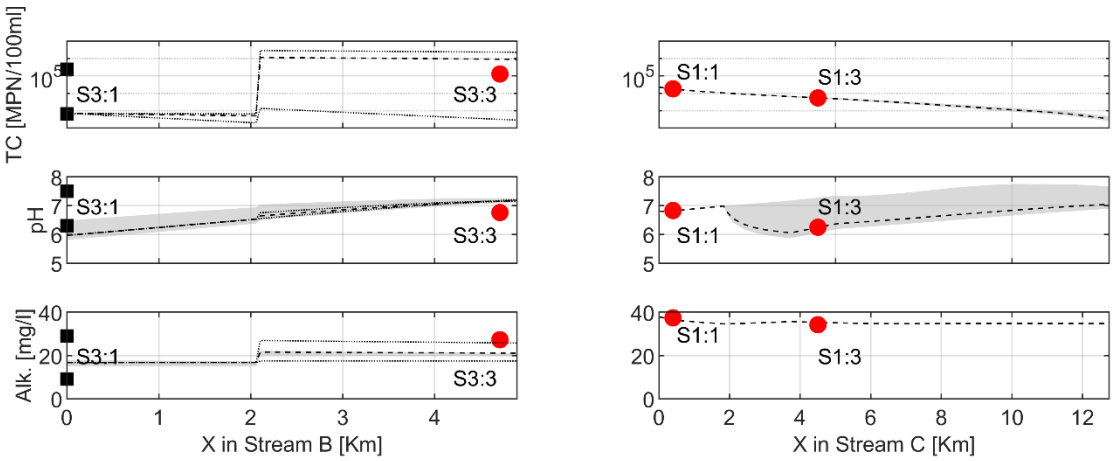

Figure S5.10. Calibration of pathogens, pH and alkalinity – Streams B and C.

S6. Model verification plots

Figure S6.1. Legend.

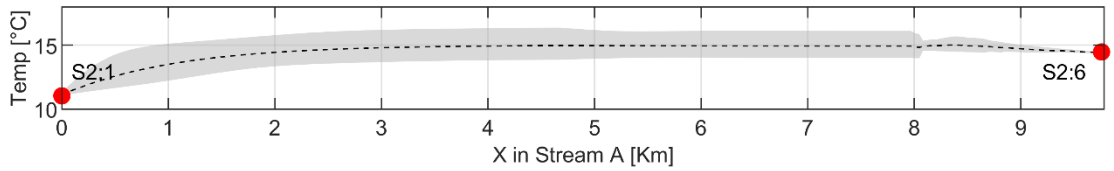

Figure S6.2. Verification of temperature – Stream A.

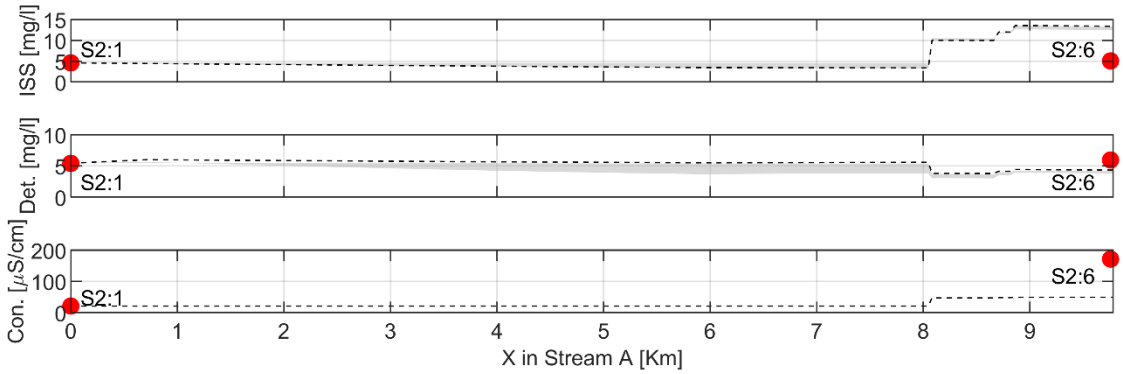

Figure S6.3. Verification of solids and conductivity – Stream A.

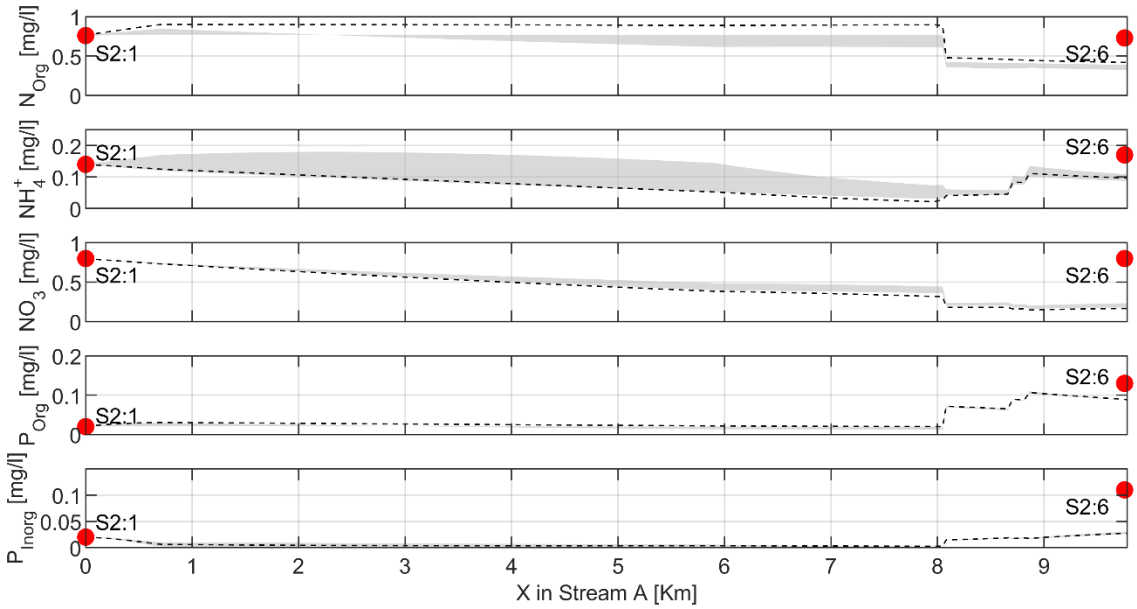

Figure S6.4. Verification of Nutrients – Stream A.

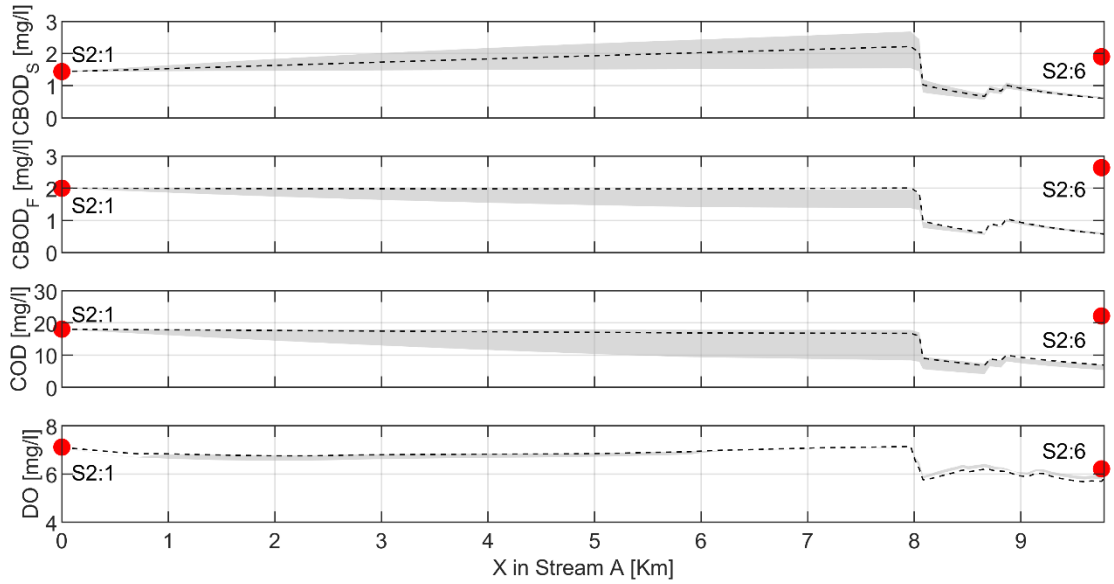

Figure S6.5. Verification of dissolved oxygen and its demanding constituents – Stream A.

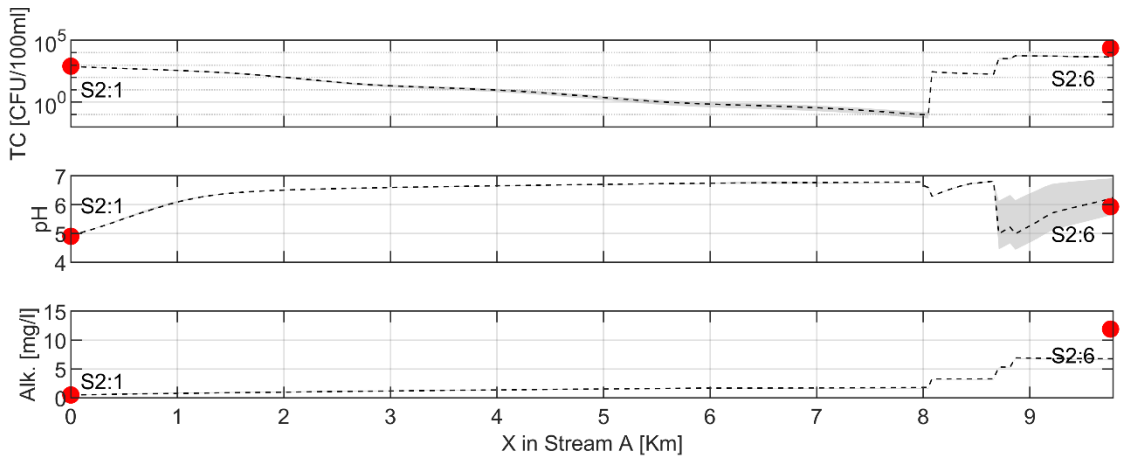

Figure S6.6. Validation of pathogens, pH and alkalinity – Stream A.

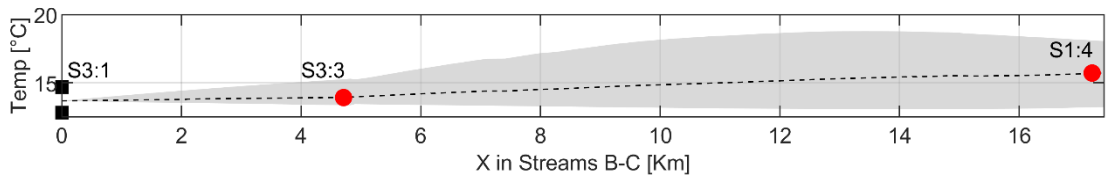

Figure S6.7. Verification of temperature – Streams B and C.

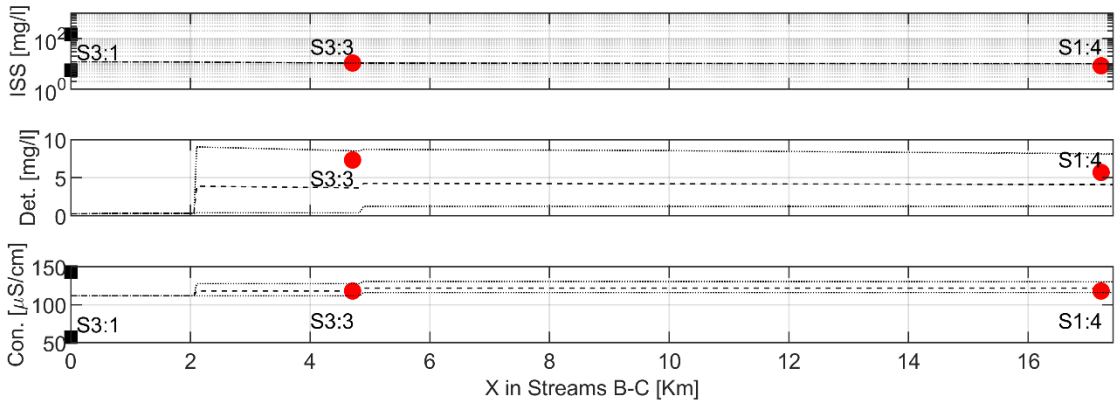

Figure S6.8. Verification of solids and conductivity – Streams B and C.

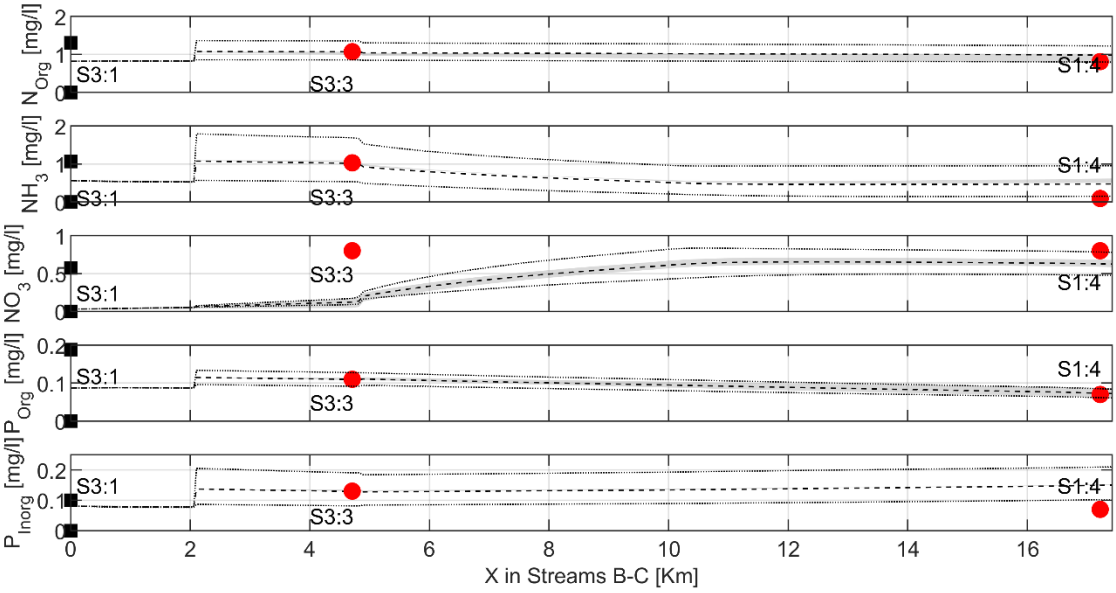

Figure S6.9. Verification of nutrients – Streams B and C.

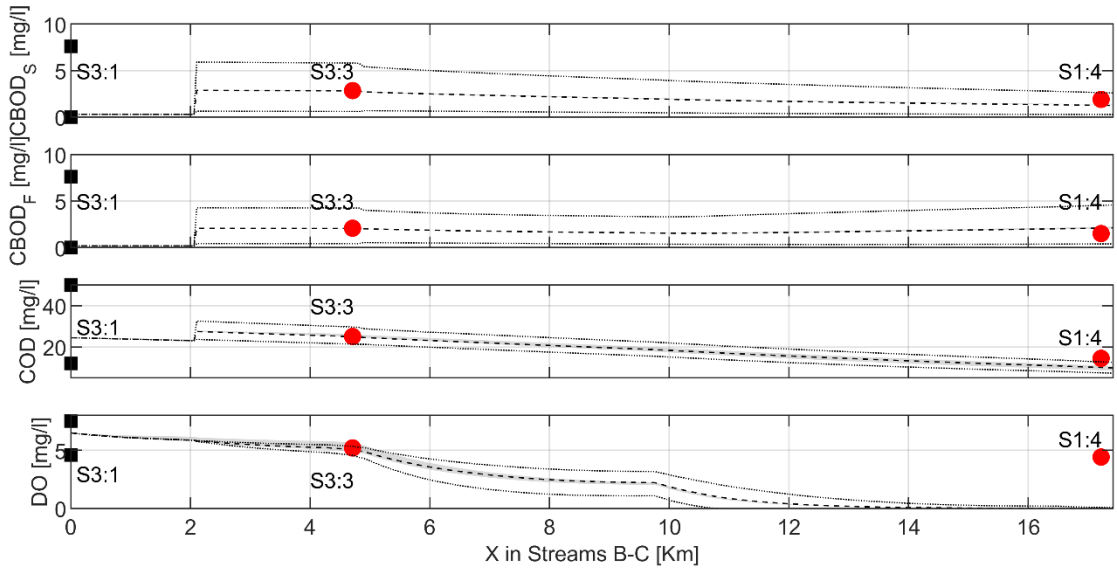

Figure S6.10. Verification of dissolved oxygen and its demanding constituents – Streams B and C.

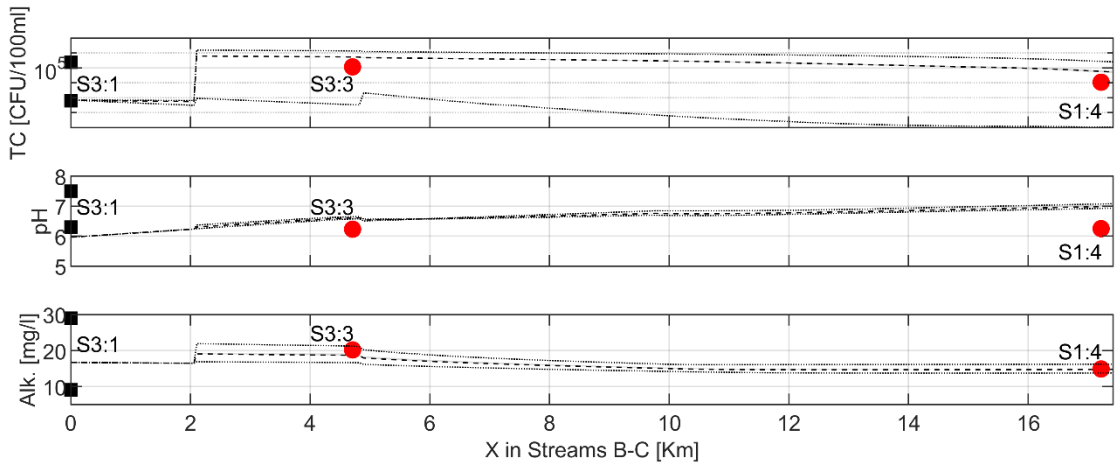

Figure S6.11. Verification of pathogens, pH and alkalinity – Streams B and C.

S7. Parametric uncertainty

Table S7.1 Values and sensitivity analysis for state variables and parameters of the model

Group	State variable	Parameter	Values: Optimal (Quantile 2.5, Quantile 97.5)			
			Stream A (segment 1) [1]	Stream A (segment 2) [2]	Stream B	Stream C
Solids	ISS	vss	0.084 (0.002, 0.098)	0.072 (0.060,0.079)	1.888 (1.513,1.987)	0.105 (0.013,0.165)*
	Det	kdt	0.091 (0.010, 0.184)*	0.108 (0.103,0.198)*	0.813 (0.806,0.993)	0.055 (0.051,0.188)*
		vdt	0.013 (0.004,0.095)*	0.014 (0.010,0.020)	0.665 (0.559,0.747)	0.050 (0.005,0.050)*
Organic matter & Pathogens	$CBOD_S$	khc	0.039 (0.001, 0.069)	0.776 (0.725, 1.096)*	1.074(0.760, 1.095)	1.986 (1.775, 2.092)*
		kdcs	0.064 (0.002, 0.067)	1.972 (1.536, 1.993)	0.521(0.508, 0.985)	2.028 (1.791, 2.094)
	$CBOD_F$	kdc	0.007 (0.002, 0.128)*	3.288 (3.014, 3.294)	1.811(1.047, 1.974)	6.580 (6.078, 6.596)*
	COD	kgen	0.003 (0.002, 0.133)*	1.622 (1.412,1.787)	2.163 (1.618, 2.191)	3.017 (2.935, 3.259)*
		vgen	0.018 (0.002, 0.136)*	0.024 (0.010,0.030)	0.491 (0.113,0.494)	0.037 (0.009,0.184)*
	TC	kpath	0.158 (0.006, 0.194)	0.318 (0.059,0.391)*	1.826 (1.520, 1.995)	1.275 (1.034, 1.388)*
		vpath	0.053 (0.007, 0.194)	0.118 (0.014, 0.145)	1.519 (1.518, 1.988)	1.187 (1.033, 1.370)
Nutrients	N_{org}	khn	0.008 (0.001, 0.091)*	0.246 (0.210, 0.354)*	0.043 (0.018, 0.779)	0.105 (0.069, 0.330)*
		von	0.015 (0.001, 0.092)*	0.017 (0.010, 0.020)	0.070 (0.015, 0.763)	0.052 (0.051, 0.274)*
	NH_4^+	kn	0.340 (0.310, 0.779)*	1.643 (1.512, 1.968)*	1.834 (0.196, 2.758)*	9.020 (8.590, 9.144)*
	P_{org}	khp	0.093 (0.007, 0.278)*	0.423 (0.405, 0.514)	0.227 (0.006, 0.638)	0.517 (0.324, 0.725)*
		vop	0.044 (0.003, 0.135)*	0.407 (0.402, 0.553)	0.800 (0.030, 0.992)	0.513 (0.373, 0.677)*
	P_{inorg}	vip	0.063 (0.004, 0.145)	0.101 (0.056, 0.196)	1.883 (0.370, 1.992)	0.068 (0.002, 0.178)*
Plants & algae	Phyto	kga	2.2801 (2.021, 2.944)*	2.275 (2.202, 2.297)	2.201 (1.539, 2.961)	2.289 (2.016, 2.396)
		krea	0.2403 (0.051, 0.394)*	0.252 (0.201, 0.268)	0.201 (0.026, 0.391)	0.108 (0.069, 0.394)
		kdea	0.1959 (0.021, 0.196)*	0.114 (0.052, 0.146)	0.232 (0.012, 0.242)	0.002 (0.001, 0.192)
		va	0.1305 (0.015, 0.195)	0.072 (0.070, 0.080)	0.165 (0.018, 0.197)	0.185 (0.008, 0.197)
	BotP	kgaF	4.470 (2.927, 19.487)	8.087 (8.079, 11.906)	7.605 (2.786, 19.49)	8.253 (5.072, 14.24)*
		krea1F	0.166 (0.153, 0.247)	0.154 (0.153, 0.247)	0.227 (0.144, 0.247)	0.395 (0.131, 0.396)
		krea2f	0.550 (0.551, 0.608)	0.587 (0.504, 0.603)	0.585 (0.503, 0.608)	0.593 (0.552, 0.607)
		kexaF	0.124 (0.104, 0.245)	0.122 (0.103, 0.199)	0.149 (0.104, 0.247)	0.129 (0.103, 0.196)
		kdeaF	0.286 (0.017, 0.343)	0.102 (0.103, 0.196)	0.212 (0.016, 0.336)	0.107 (0.103, 0.190)
		Nbmin	8.640 (5.074, 9.821)	7.559 (7.018, 7.975)	7.508 (5.092, 9.850)	7.150 (7.019, 7.587)
		Pbmin	3.003 (2.062, 3.966)	3.2085 (2.920, 3.291)	2.132 (2.038, 3.930)	3.312 (2.832, 3.384)
		Nupmax	359.0 (341.6, 378.8)	343.9 (341.0, 379.1)	353.3 (341.7, 379.2)	366.3 (341.5, 368.8)
		Pupmax	96.57 (71.03, 109.2)	85.61 (80.28, 89.67)	96.72 (71.21, 109.4)	83.64 (80.44, 89.93)
		KNratio	2.219 (1.155, 2.484)	1.195 (1.101, 1.293)	1.868 (1.156, 2.477)	1.173 (1.113, 1.292)
		KPratio	1.618 (1.279, 1.780)	1.661 (1.506, 1.694)	1.250 (1.215, 1.784)	1.561 (1.417, 1.686)

[1] Comprised between sites S2:1 and S2:2; [2] comprised between sites S2:3 and S2:6; * refers to sensitive parameters.

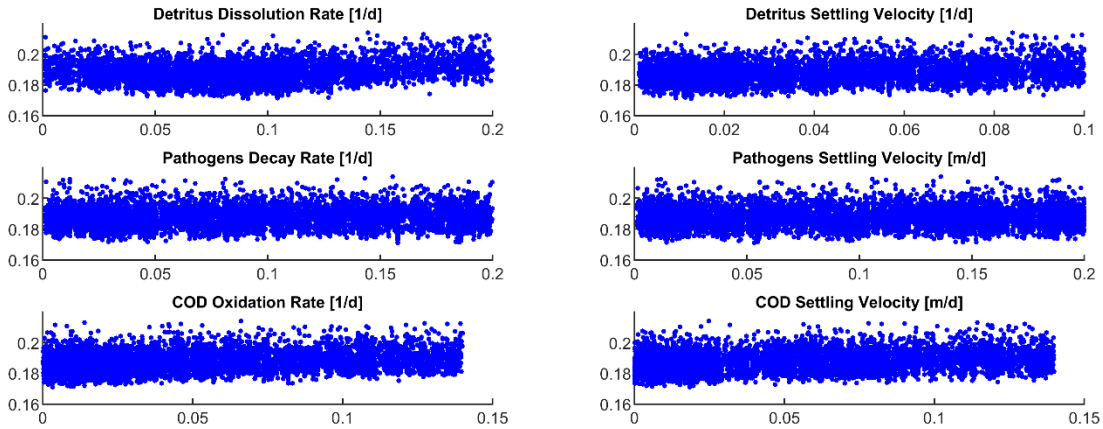

Figure S7.1. Dotty plots for Detritus, Pathogens and COD parameters – Stream A (S2-1 to S2-2).

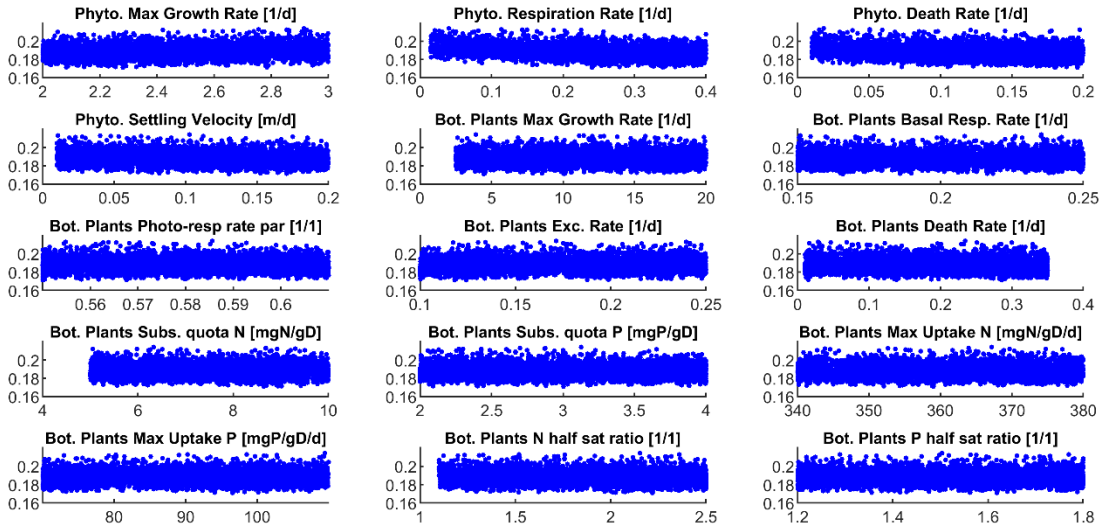

Figure S7.2. Dotty plots for phytoplankton and bottom plants parameters – Stream A (S2-1 to S2-2).

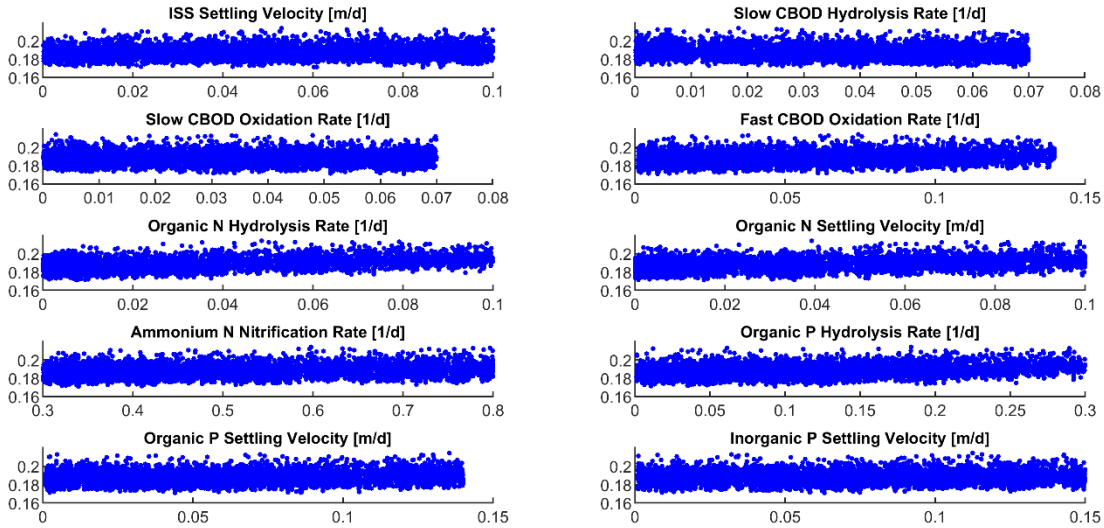

Figure S7.3. Dotty plots for ISS, CBOD and nutrient parameters - Stream A (S2-1 to S2-2).

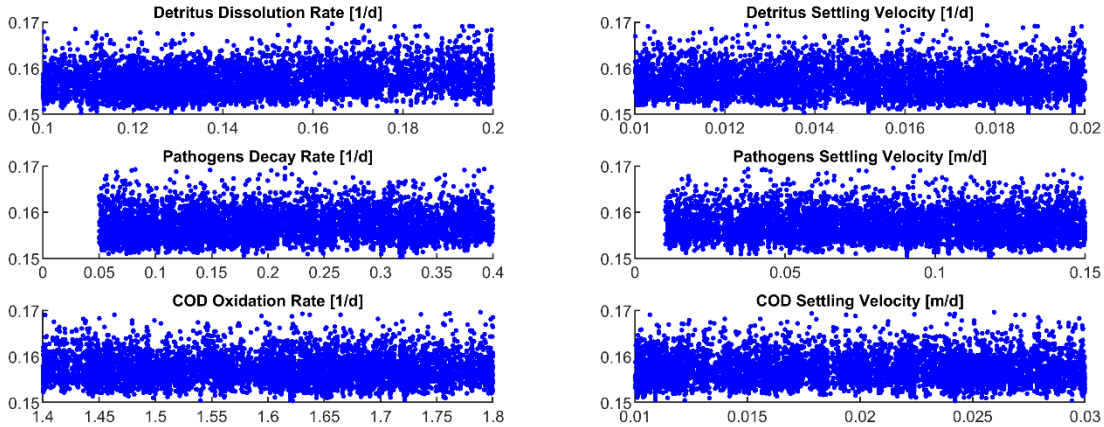

Figure S7.4. Dotty plots for Detritus, Pathogens and COD parameters – Stream A (S2-3 to S2-6).

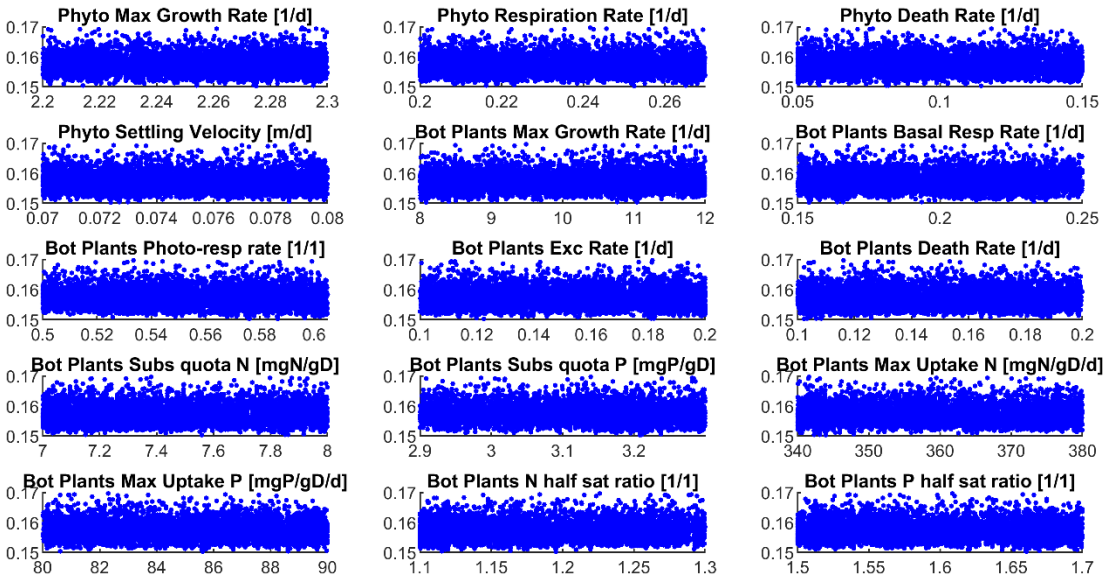

Figure S7.5. Dotty plots for phytoplankton and bottom plants parameters – Stream A (S2-3 to S2-6).

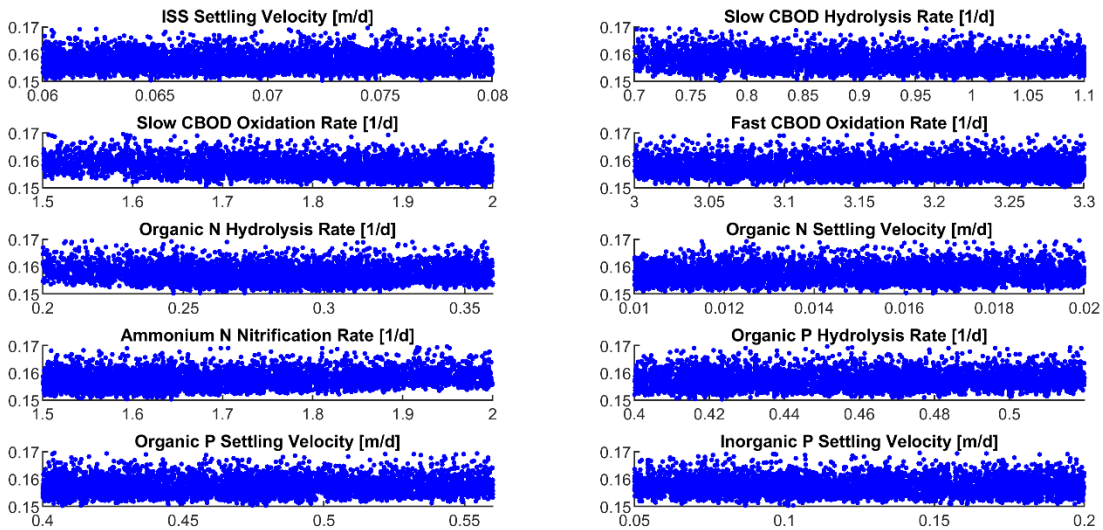

Figure S7.6. Dotty plots for ISS, CBOD and nutrient parameters – Stream A (S2-3 to S2-6).

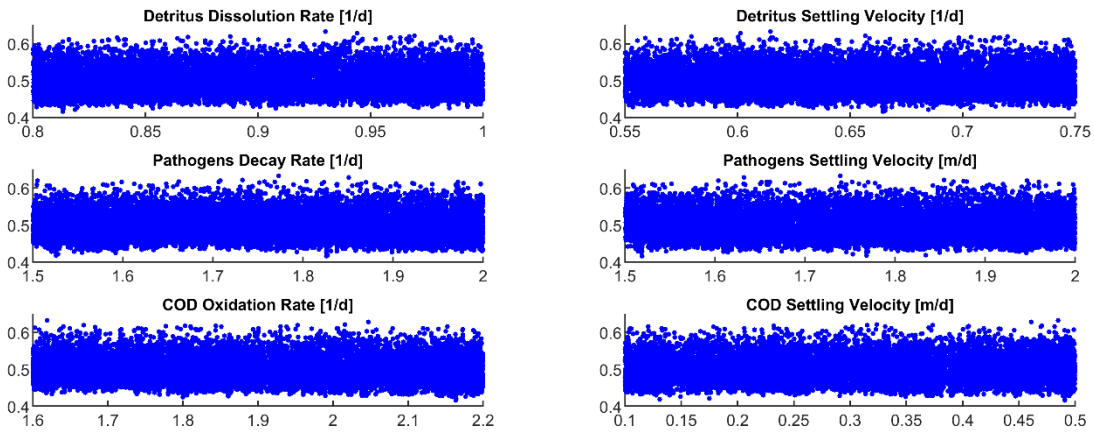

Figure S7.7. Dotty plots for Detritus, Pathogens and COD parameters – Stream B.

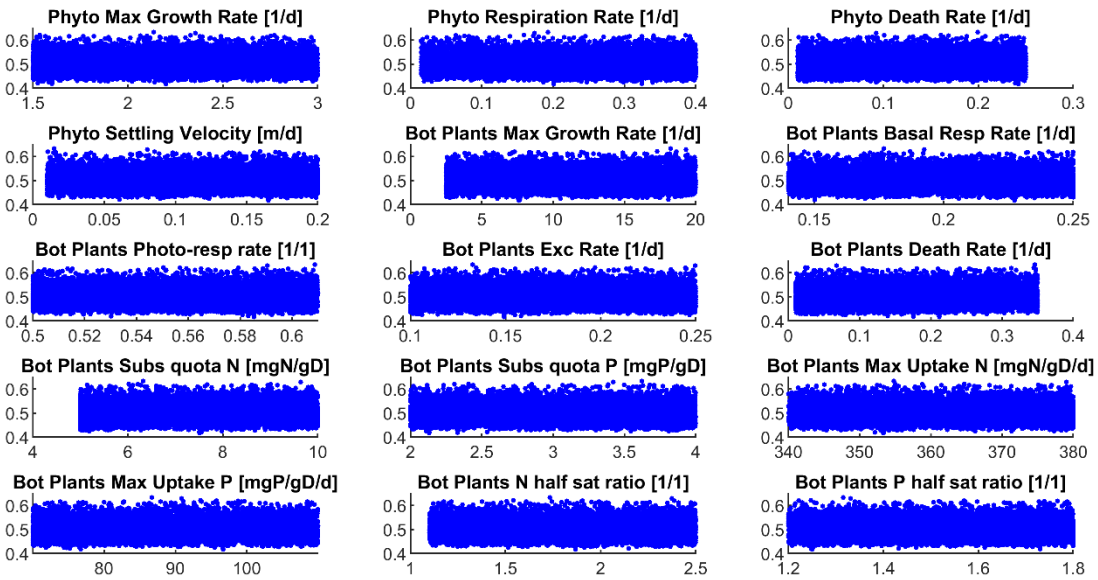

Figure S7.8. Dotty plots for phytoplankton and bottom plants parameters – Stream B.

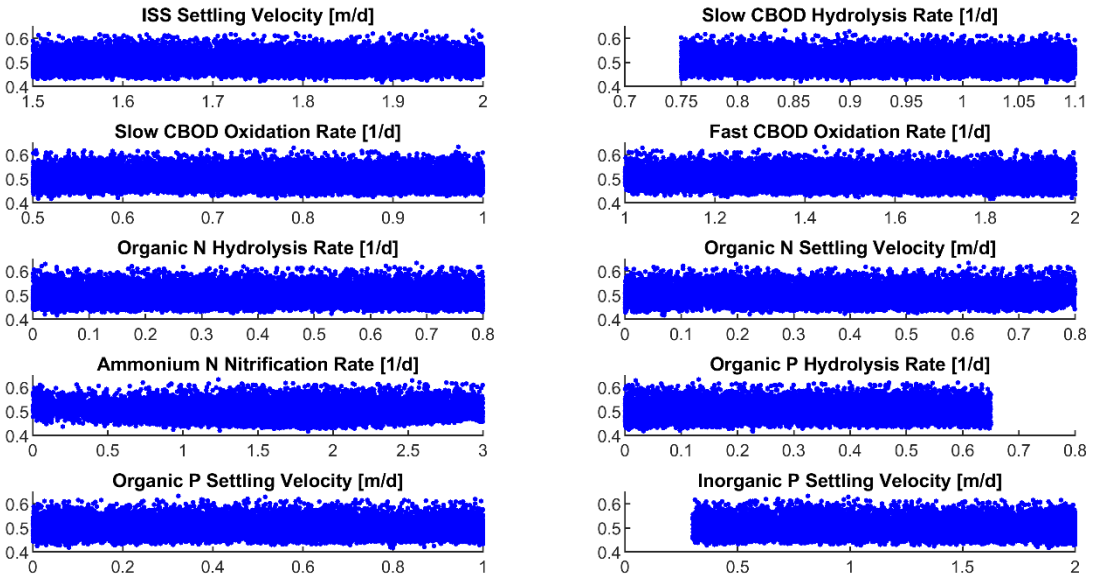

Figure S7.9. Dotty plots for ISS, CBOD and nutrient parameters – Stream B.

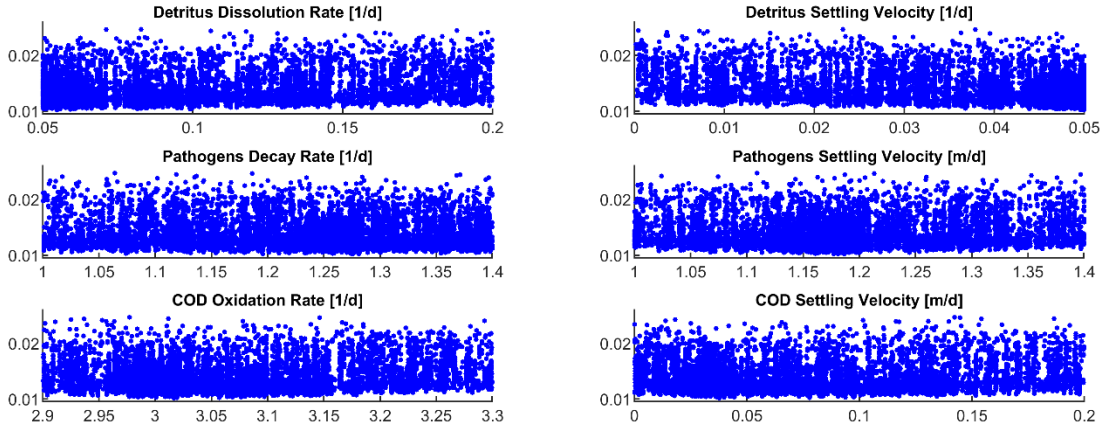

Figure S7.10. Dotty plots for Detritus, Pathogens and COD parameters – Stream C.

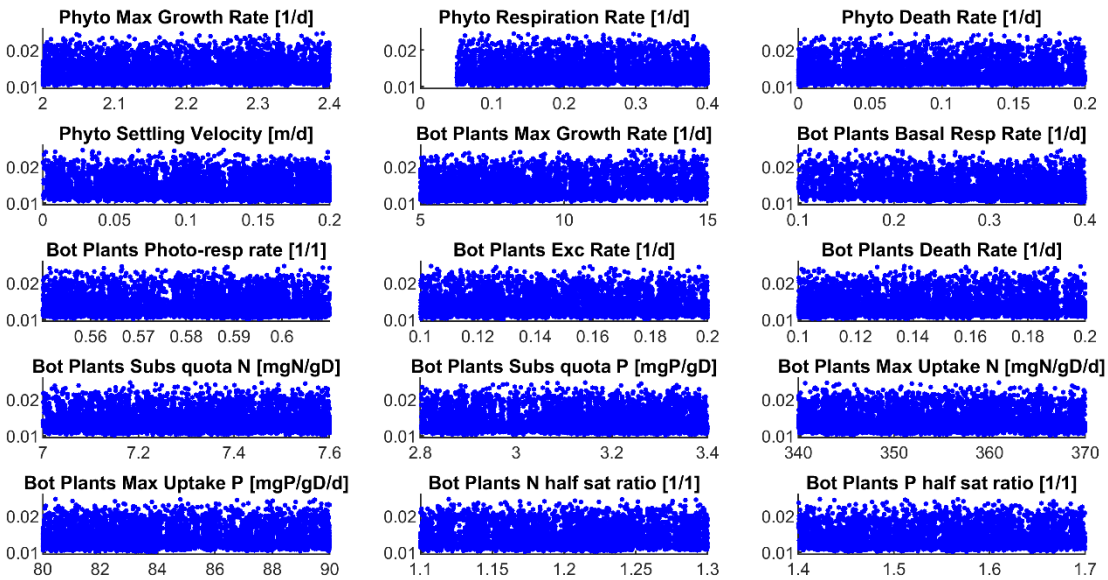

Figure S7.11. Dotty plots for phytoplankton and bottom plants parameters – Stream C.

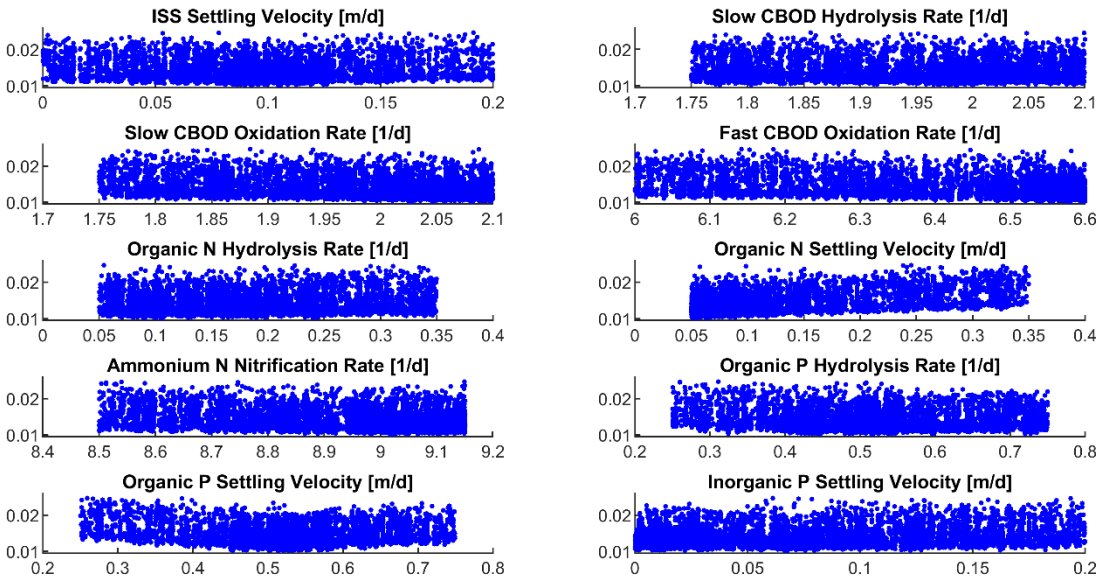

Figure S7.12. Dotty plots for ISS, CBOD and nutrient parameters – Stream C.

S8. Simulation of critical scenario

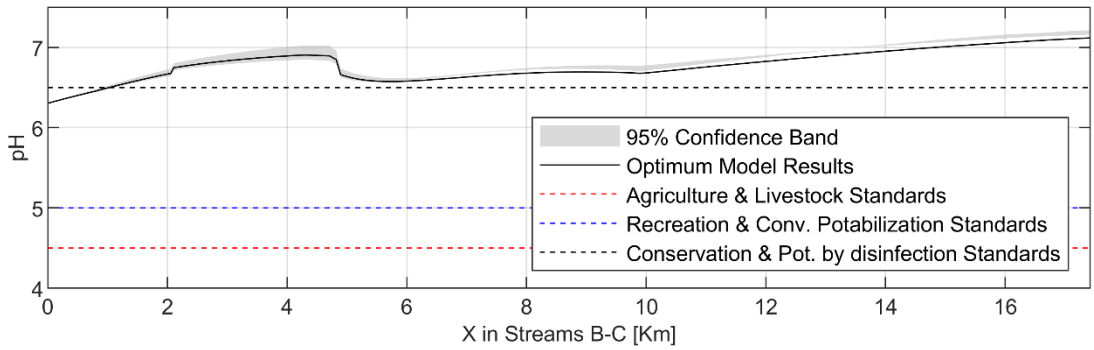

Figure S8.1. Model results for pH in critical scenario.

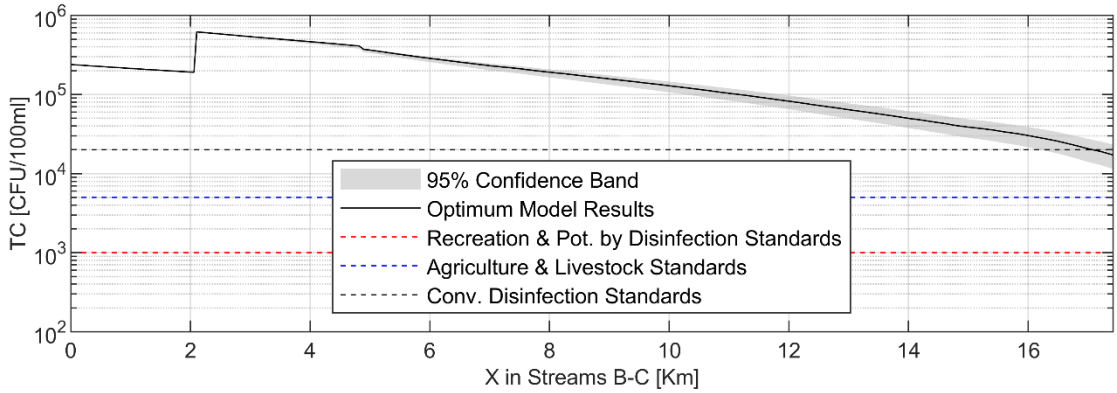

Figure S8.2. Model results for Total Coliforms in critical scenario.

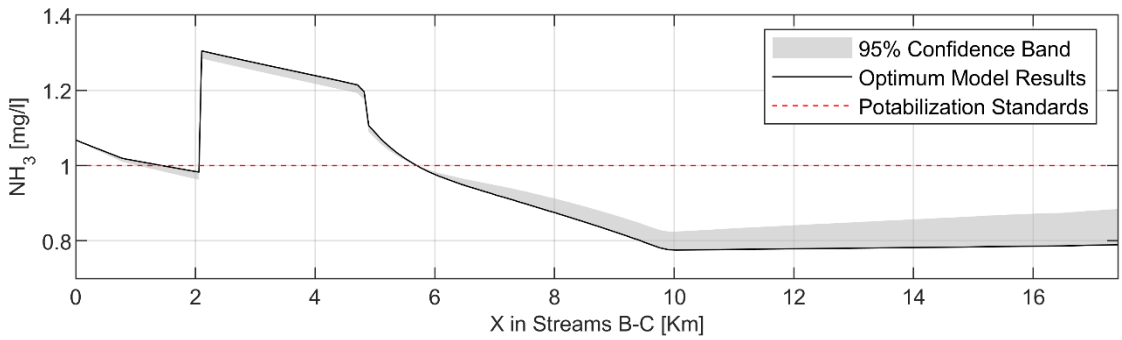

Figure S8.3. Model results for Ammonia Nitrogen in critical scenario.

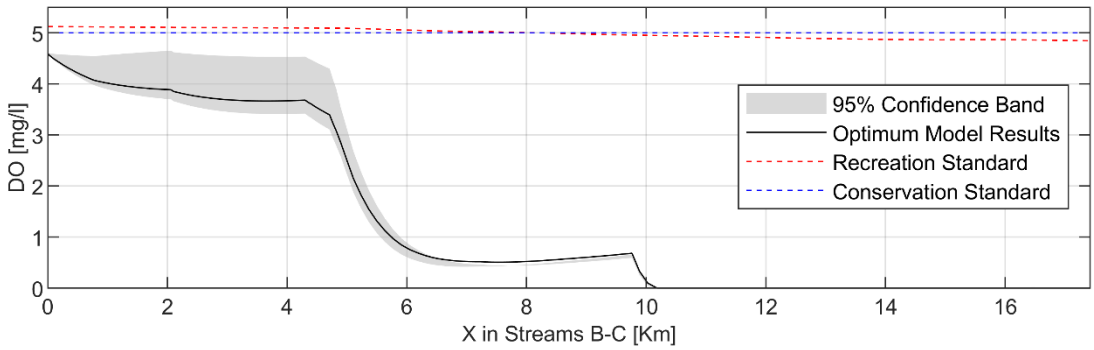

Figure S8.4. Model results for Dissolved Oxygen in critical scenario.

S9. Simulation of alternative scenario 1

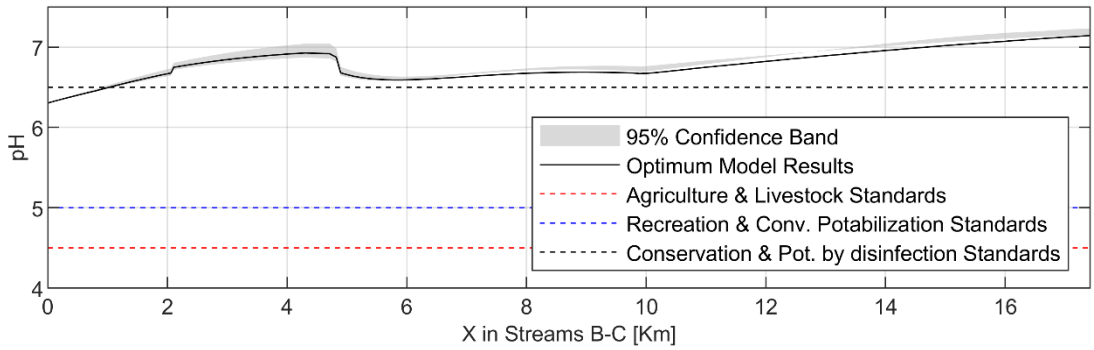

Figure S9.1. Model results for pH in alternative scenario 1.

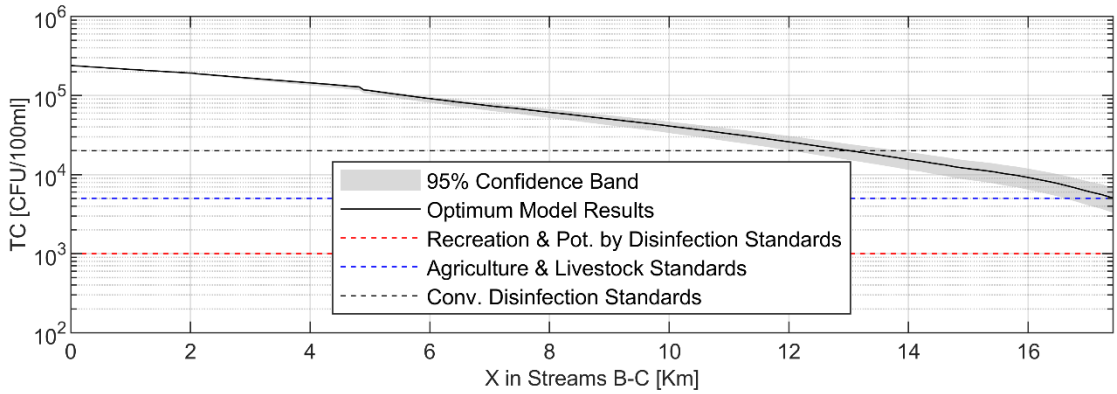

Figure S9.2. Model results for Total Coliforms in alternative scenario 1.

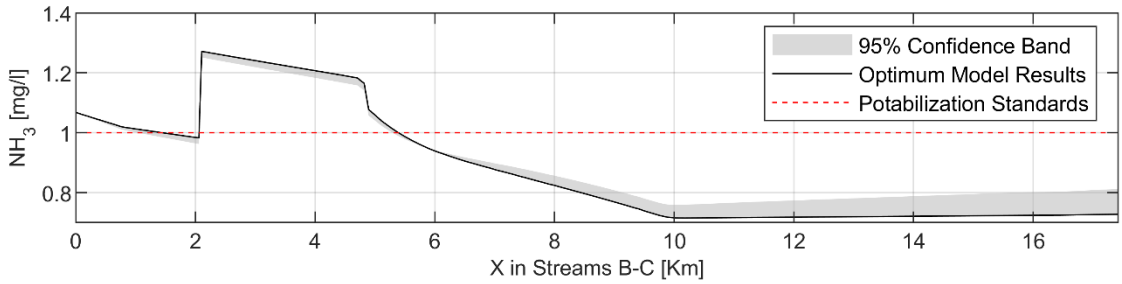

Figure S9.3. Model results for Ammonia Nitrogen in alternative scenario 1.

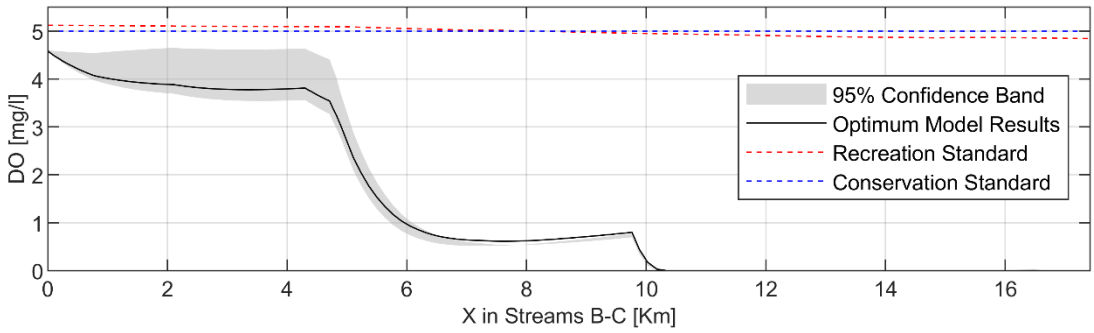

Figure S9.4. Model results for Dissolved Oxygen in alternative scenario 1.

S10. Simulation of alternative scenario 2

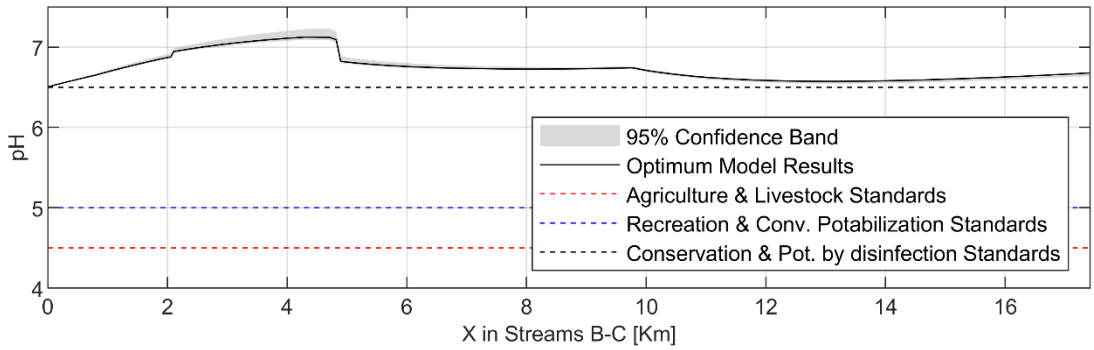

Figure S10.1. Model results for pH in alternative scenario 2.

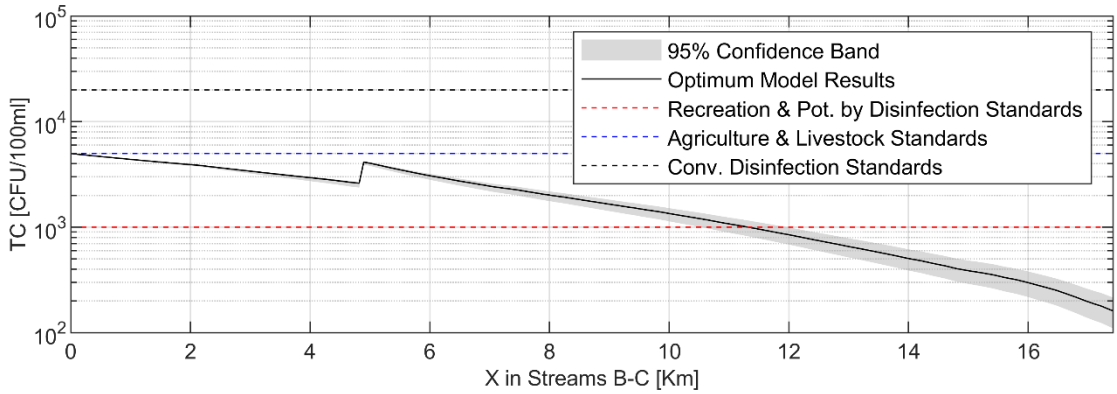

Figure S10.2. Model results for Total Coliforms in alternative scenario 2.

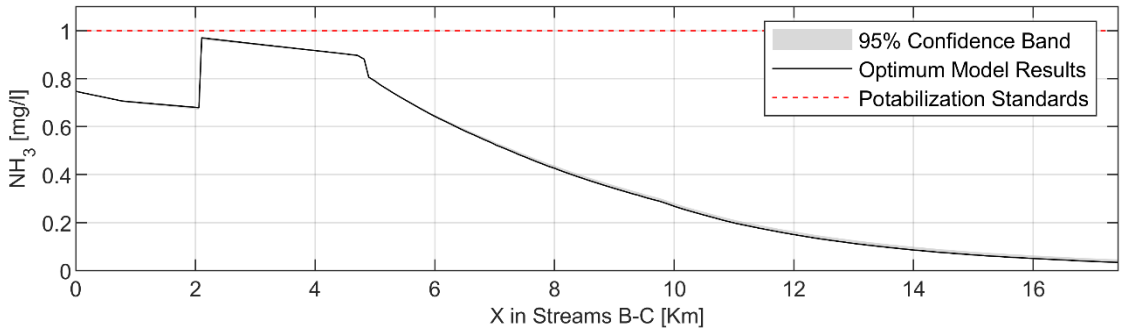

Figure S10.3. Model results for Ammonia Nitrogen in alternative scenario 2.

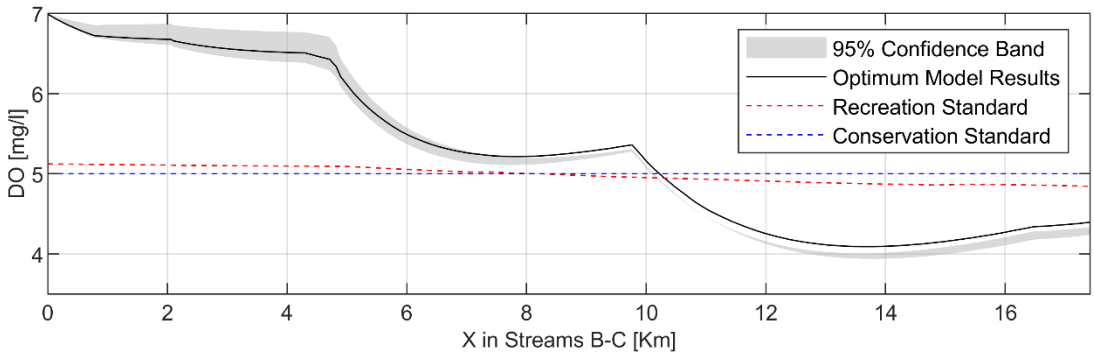

Figure S10.4. Model results for Dissolved Oxygen in alternative scenario 2.