Appendix 11. Model Archival Summary for Chloride Concentration at U.S. Geological Survey Site 06887500, Kansas River at Wamego, Kansas, during July 2012 through September 2019

This model archival summary summarizes the chloride (Cl; U.S. Geological Survey [USGS] parameter code 00940) concentration model developed to compute 15-minute Cl concentrations from July 2012 onward. This model supersedes all previous models.

Any use of trade, firm, or product names is for descriptive purposes only and does not imply endorsement by the U.S. Government.

Site and Model Information

Site number: 06887500
Site name: Kansas River at Wamego, Kansas
Location: Lat 39°11'54", long 96°18'19" referenced to North American Datum of 1927, in SW 1/4 NW 1/4 SE 1/4 sec.9, T.10 S., R.10 E., Pottawatomie County, Kans., hydrologic unit 10270102.

Equipment: A YSI 6600 water-quality monitor equipped with sensors for water temperature, specific conductance (SC), dissolved oxygen, pH, and turbidity was installed from August 2012 through June 2014. A Xylem YSI EXO2 water-quality monitor equipped with sensors for water temperature, SC, dissolved oxygen, pH, turbidity, and chlorophyll and phycocyanin fluorescence was installed during June 2014 through September 2019. The monitor was housed in a 4-inch-diameter galvanized steel pipe. Readings from the water-quality monitor were recorded every 15 minutes and transmitted by way of satellite, hourly.

Date model was created: March 30, 2020

Model calibration data period: July 19, 2012, through September 23, 2019

Model application date: July 19, 2012, onward

Model-Calibration Dataset

All data were collected using USGS protocols (Wagner and others, 2006; U.S. Geological Survey, variously dated) and are stored in the National Water Information System (U.S. Geological Survey, 2020) database and available to the public. Ordinary least squares analysis was used to develop regression models using R programming language (R Core Team, 2020). Potential explanatory variables that were evaluated individually and in combination included streamflow, water temperature, SC, dissolved oxygen, pH, turbidity, and chlorophyll and phycocyanin fluorescence. The maximum time span between two continuous data points used for interpolation was 2 hours (in order to preserve the sample dataset, field monitor averages obtained during sample collection were used for model development data if no continuous data were available or if gaps larger than 1 hour in the continuous data record resulted in missing interpolated data). Seasonal components (sine and cosine variables) were also evaluated as potential explanatory variables.

The final selected regression model was based on 101 concurrent measurements of Cl concentration and sensor-measured SC during July 19, 2012, through September 23, 2019. Samples were collected throughout the range of continuously observed hydrologic conditions. No samples had concentrations below laboratory detection limits. Summary statistics and the complete model-calibration dataset are provided below. Potential outliers were identified using the methods described in Rasmussen and others (2009). Additionally, studentized residuals from the final model were inspected for values greater than three or less than negative three. Values outside of that range were considered potential outliers and were investigated. One of the sensor-measured SC samples, from July 28, 2014, was deemed an outlier and removed from the model calibration dataset. The removed sensor-measured SC value was significantly lower than the field monitor and laboratory result during this sample. All other potential outliers were not found to have errors associated with collection, processing, or analysis and were therefore considered valid.

This model is specific to the Kansas River at Wamego, Kans., during this study period and cannot be applied to data collected from other sites on the Kansas River or data collected from other waterbodies.

Chloride Sampling Details

Cross-section samples typically were collected either from the downstream side of the bridge or instream within 100 feet of the bridge. The equal-width-increment collection method was used (although multiple vertical, single vertical, and grab samples were occasionally collected), and samples typically were composited for analysis (U.S. Geological Survey, variously dated). During July 2012 through June 2017, cross-section samples were collected every 2 weeks during March through October, once a month during November through February, and during selected reservoir release and runoff events. During July 2017 through September 2019, cross-section samples were collected on a monthly to bimonthly basis, depending on flow conditions. A FISP US DH–81, DH–95,

D–95, D–96a, or D–96 depth integrating sampler was used. Additional detail on sample collection is available in Foster and Graham (2016) and Graham and others (2018). Samples were analyzed for Cl concentration at the USGS National Water Quality Laboratory in Lakewood, Colorado.

Model Development

Ordinary least squares regression analysis was done using R programming language (R Core Team, 2020) to relate discretely collected Cl concentration to sensor-measured SC. The distribution of residuals was examined for normality, and the plots of residuals (the difference between the measured and computed values) were examined for homoscedasticity (departures from zero did not change substantially over the range of computed values). Previously published explanatory variables were also strongly considered for continuity.

SC was selected as a good surrogate for Cl based on residual plots, coefficient of determination (R^2), and model standard percentage error. Values for all the aforementioned statistics were computed and are included below along with all relevant sample data and additional statistical information.

Model Summary

The following is a summary of final regression analysis for Cl concentration at USGS site 06887500:

Cl concentration-based model:

$$\log Cl = 1.77 \times \log SC - 3.22$$

where

log = logarithm base 10;

Cl = chloride concentration, in milligrams per liter; and

SC = specific conductance, in microsiemens per centimeter at 25 degrees Celsius.

SC makes physical and statistical sense as an explanatory variable for Cl because of its positive correlation with charged ionic species (Hem, 1992).

The logarithmically (log) transformed model may be retransformed to the original units so that Cl can be calculated directly. The retransformation introduces a bias in the calculated constituent. This bias may be corrected using Duan's bias correction factor (BCF; Duan, 1983). For this model, the calculated BCF is 1.01. The retransformed model, accounting for BCF is as follows:

$$Cl = 1.01 \times (SC^{1.77} \times 10^{-3.22})$$

Previous Models

Start Year	End Year	Model Equation	Reference
2012	2019	logCl = 1.82logSC - 3.33	Foster and Graham (2016)
1999	2003	logCl = 1.60logSC - 2.73	Rasmussen and others (2005)

Model Statistics, Data, and Plots

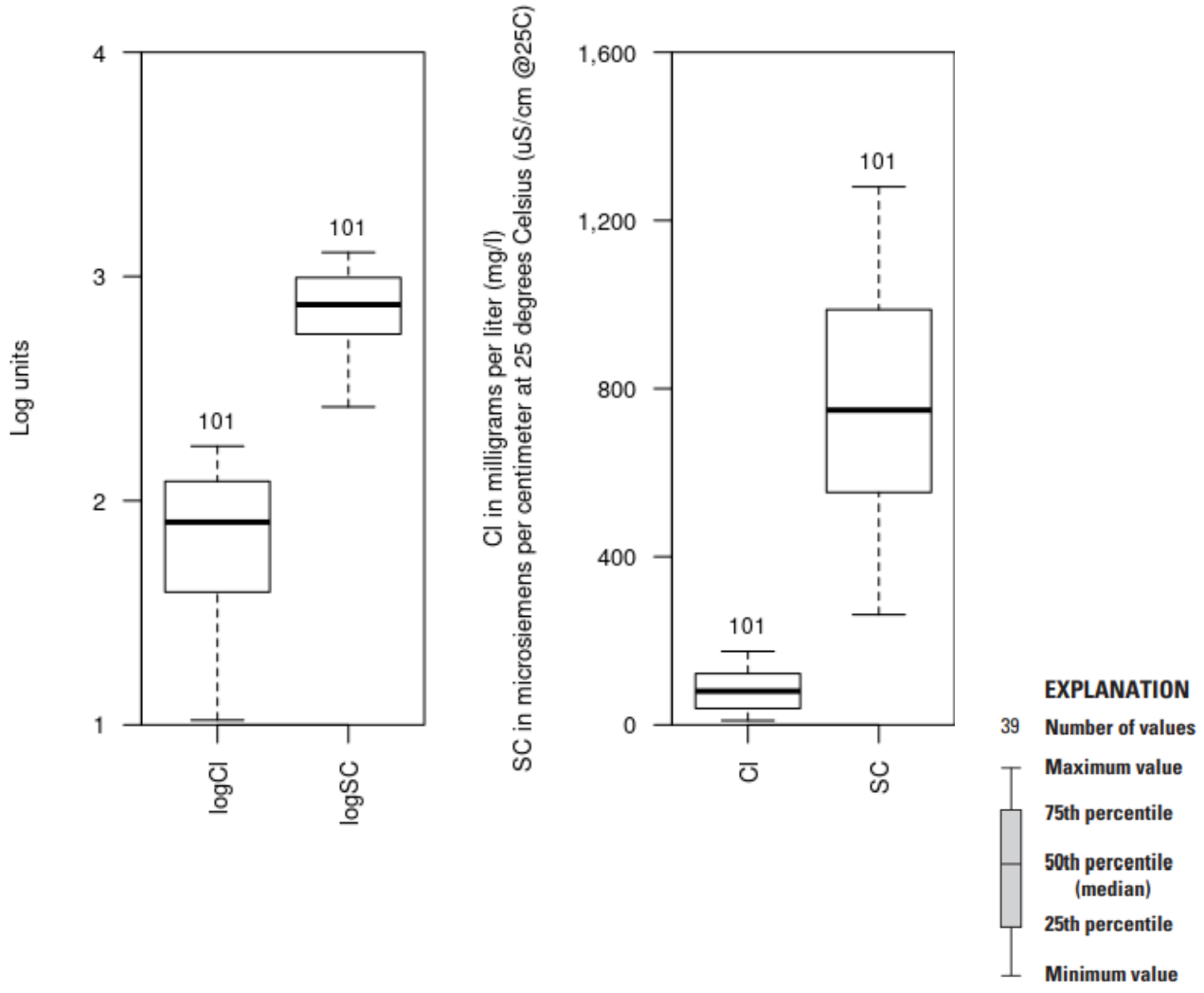
Model

logCl = + 1.77 * logSC - 3.22

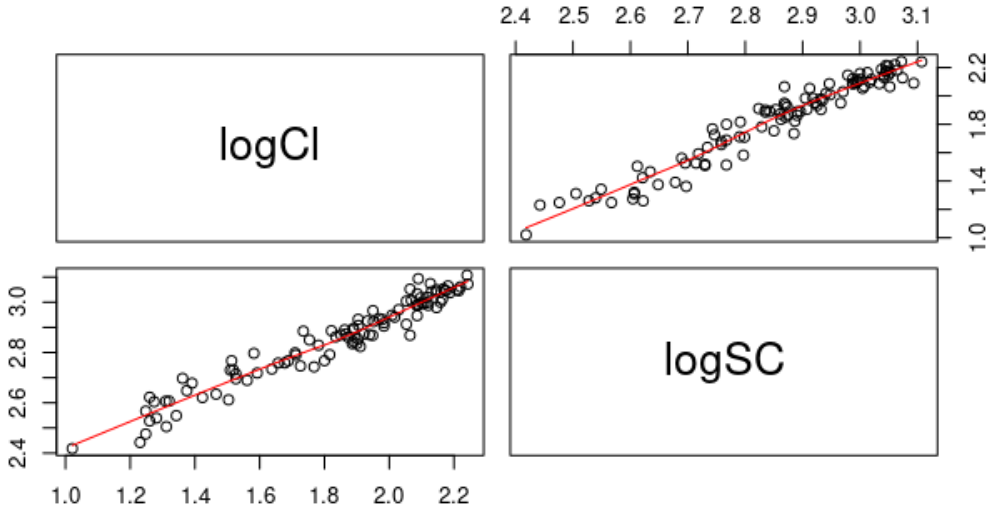
Variable Summary Statistics

	logCl	Cl	logSC	SC
Minimum	1.02	10.5	2.42	262
1st Quartile	1.59	39.1	2.74	553
Median	1.90	80.2	2.87	749
Mean	1.83	82.8	2.85	762
3rd Quartile	2.09	122.0	2.99	988
Maximum	2.24	175.0	3.11	1280

Box Plots



Exploratory Plots



Red line shows the locally weighted scatterplot smoothing (LOWESS).

The x- and y-axis labels for a given bivariate plot are defined by the intersecting row and column labels.

Basic Model Statistics

Number of Observations	101
Standard error (RMSE)	0.0755
Average Model standard percentage error (MSPE)	17.5
Coefficient of determination (R^2)	0.94
Adjusted Coefficient of Determination (Adj. R^2)	0.939
Bias Correction Factor (BCF)	1.01

Explanatory Variables

	Coefficients	Standard Error	t value	Pr(>|t|)
(Intercept)	-3.22	0.128	-25.1	1.21e-44
logSC	1.77	0.045	39.4	2.90e-62

Correlation Matrix

	Intercept	E.vars
Intercept	1.000	-0.998
E.vars	-0.998	1.000

Outlier Test Criteria

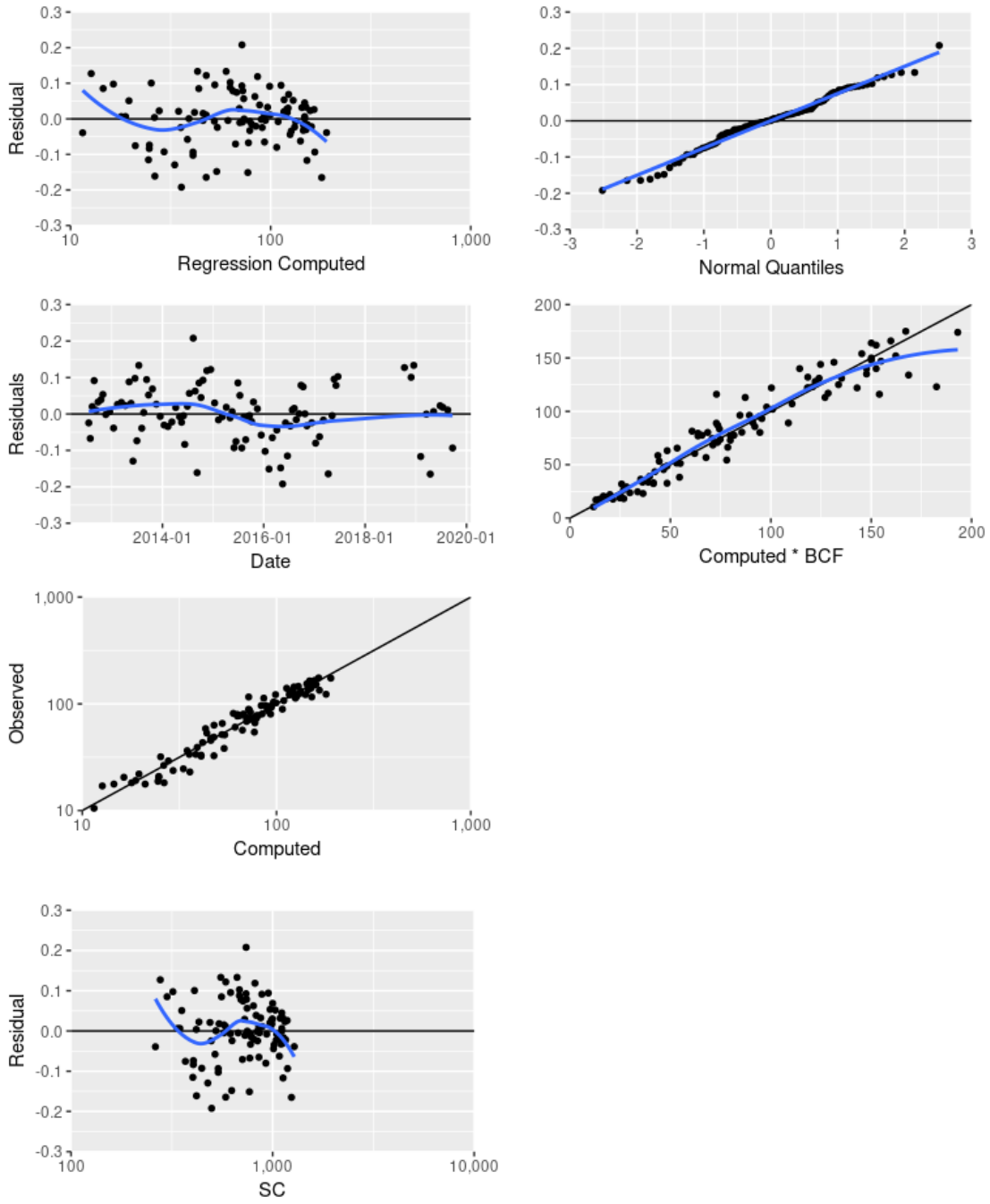
Leverage	Cook's D	DFFITS
0.0594	0.1944	0.2814

Flagged Observations

	logCl	Estimate	Residual	Standard Residual	Studentized Residual	Leverage	Cook's D	DFFITS
201306170830	1.31	1.21	0.0977	1.330	1.330	0.05270	0.0492	0.315
201308050730	1.02	1.06	-0.0392	-0.541	-0.539	0.07680	0.0122	-0.155
201408110920	2.06	1.86	0.2080	2.770	2.870	0.00999	0.0386	0.288
201409080800	1.26	1.42	-0.1610	-2.170	-2.210	0.02870	0.0694	-0.380
201506290820	1.25	1.16	0.0852	1.160	1.170	0.06020	0.0434	0.295
201605160850	1.36	1.55	-0.1920	-2.570	-2.650	0.01850	0.0622	-0.363
201606201210	1.27	1.39	-0.1150	-1.550	-1.560	0.03180	0.0395	-0.283

201810110940	1.23	1.10	0.1270	1.750	1.770	0.06960	0.1140	0.483	
201904150950	2.09	2.25	-0.1650	-2.220	-2.270	0.03040	0.0774	-0.402	

Statistical Plots



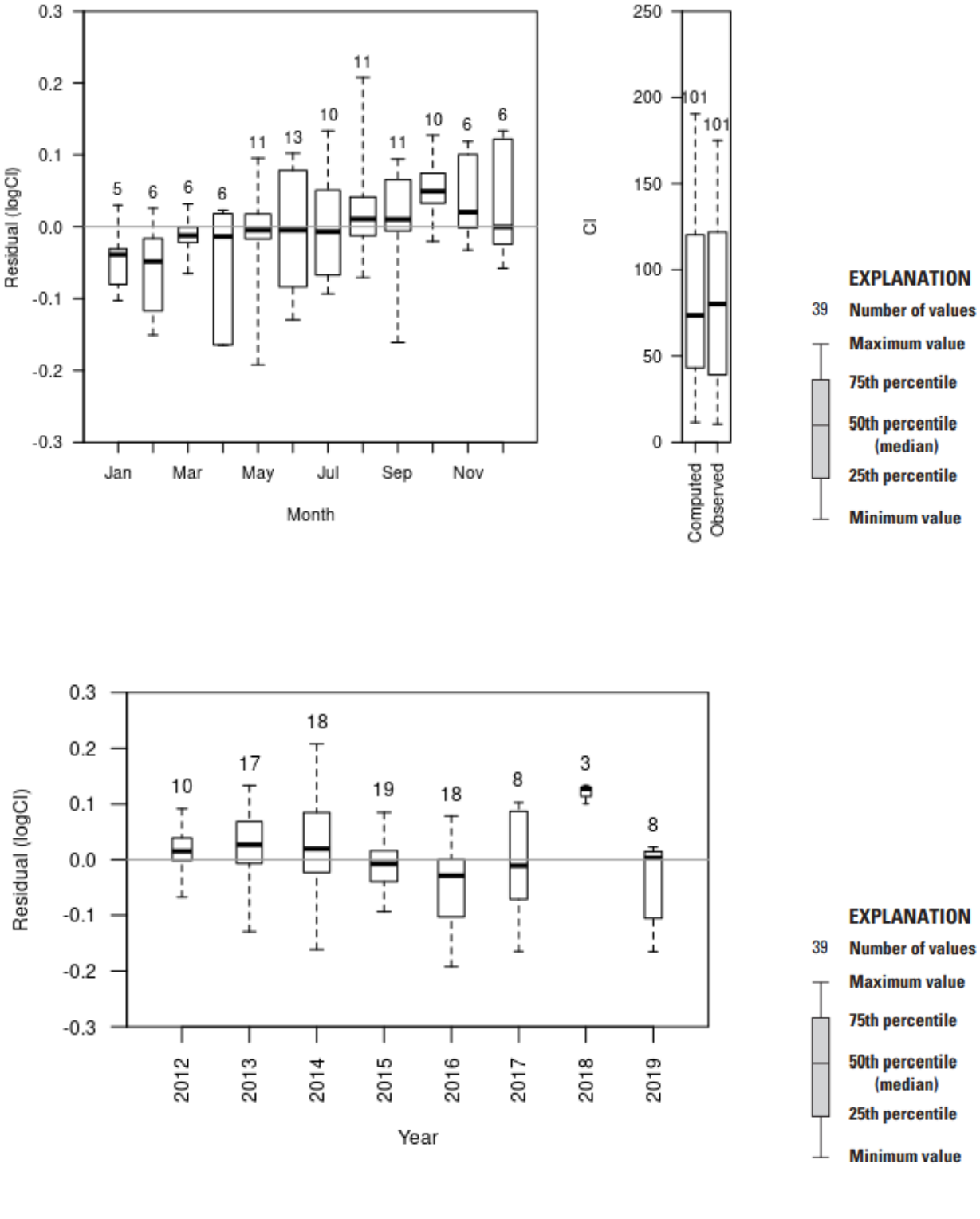
First row (left): Residual Cl related to regression computed Cl with local polynomial regression fitting, or locally estimated scatterplot smoothing (LOESS), indicated by the blue line.

First row (right): Residual Cl related to the corresponding normal quantile of the residual with simple linear regression, indicated by the blue line.

Second row: Residual Cl related to date (left) and regression computed Cl multiplied by the BCF (right) with LOESS, indicated by the blue line.

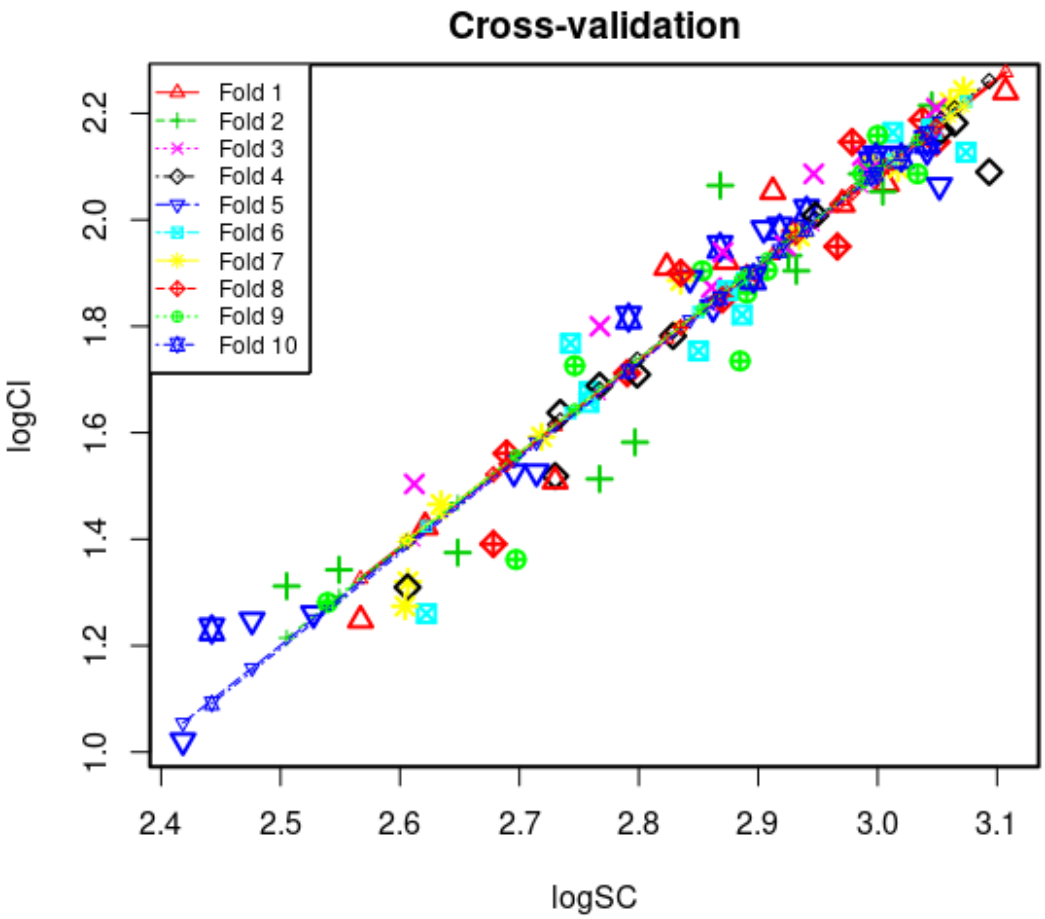
Third row: Observed Cl related to regression computed Cl.

Fourth row: Residual Cl related to SC with LOESS, indicated by the blue line.


Residual (logCI)
0.3
0.2
0.1
0.0
-0.1
-0.2
-0.3
5
6
6
6
11
13
10
11
11
10
6
6
Jan
Mar
May
Jul
Sep
Nov
Month
CI
250
200
150
100
50
0
101
101
Computed
Observed
EXPLANATION
39
Number of values
Maximum value
75th percentile
50th percentile
(median)
25th percentile
Minimum value

Residual (logCI)
0.3
0.2
0.1
0.0
-0.1
-0.2
-0.3
10
17
18
19
18
8
3
8
2012
2013
2014
2015
2016
2017
2018
2019
Year
EXPLANATION
39
Number of values
Maximum value
75th percentile
50th percentile
(median)
25th percentile
Minimum value

Cross-Validation

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Fold - equal partition of the data (10 percent of the data).

Large symbols – observed value of a data point removed in a fold.

Small symbols – recomputed value of a data point removed in a fold.

Recomputed regression lines – adjusted regression line with one fold removed.


              Minimum MSE of folds:  0.00312
                 Mean MSE of folds:  0.00574
               Median MSE of folds:  0.00496
              Maximum MSE of folds:  0.01110
 (Mean MSE of folds) / (Model MSE):  1.01000
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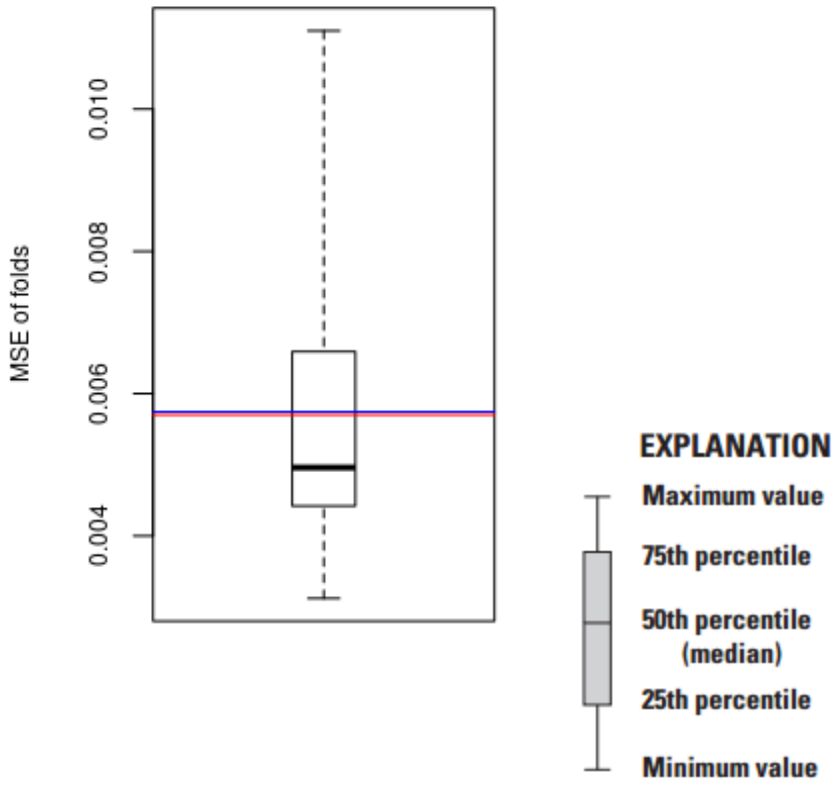

Red line - Model MSE

Blue line - Mean MSE of folds

Model-Calibration Dataset

	Date	logCl	logSC	Cl	SC	Computed logCl	Computed Cl	Residual	Normal Quantiles	Censored Values
1	2012-07-19	1.93	2.93	85.7	842	1.96	92	-0.0246	-0.546	--
2	2012-07-30	1.82	2.89	66.3	770	1.89	78.6	-0.0673	-0.901	--
3	2012-08-13	2.09	2.99	122	970	2.07	118	0.0201	0.328	--
4	2012-08-27	2.09	2.95	122	884	1.99	100	0.0914	1.15	--
5	2012-09-10	1.98	2.93	95.2	854	1.97	94.4	0.0102	0.124	--
6	2012-09-24	2.02	2.94	104	872	1.98	97.9	0.0326	0.575	--
7	2012-10-15	1.98	2.92	96.3	828	1.94	89.3	0.039	0.635	--
8	2012-10-29	2.12	2.99	132	971	2.07	118	0.0535	0.761	--
9	2012-11-19	1.95	2.92	89.4	837	1.95	91.1	-0.00164	-0.0744	--
10	2012-12-17	2.18	3.05	150	1110	2.17	150	0.00619	0.0496	--
11	2013-01-14	2.24	3.11	174	1280	2.28	193	-0.0389	-0.696	--
12	2013-02-11	2.24	3.07	175	1180	2.22	167	0.0261	0.434	--
13	2013-03-11	2.19	3.04	154	1090	2.16	145	0.0316	0.546	--
14	2013-04-08	2.22	3.06	166	1150	2.2	160	0.023	0.407	--
15	2013-05-06	1.89	2.84	76.9	684	1.8	63.7	0.0881	1.11	--
16	2013-05-20	1.87	2.86	74.6	726	1.84	70.8	0.0291	0.489	--
17	2013-06-03	1.39	2.68	24.6	477	1.52	33.6	-0.129	-1.51	--
18	2013-06-17	1.31	2.51	20.5	320	1.21	16.6	0.0977	1.37	--
19	2013-07-01	1.32	2.61	20.9	404	1.39	25.1	-0.0737	-0.978	--
20	2013-07-15	1.91	2.82	81.4	666	1.78	60.8	0.133	1.95	--

21	2013-08-05	1.02	2.42	10.5	262	1.06	11.7	-0.0392	-0.728	--
22	2013-08-19	1.42	2.62	26.5	418	1.42	26.7	0.00384	0.0248	--
23	2013-09-09	2.15	2.98	140	952	2.05	114	0.0942	1.25	--
24	2013-09-23	2.16	3.01	146	1030	2.11	131	0.0519	0.728	--
25	2013-10-21	2.16	3	144	1000	2.09	125	0.0687	0.864	--
26	2013-11-18	2.11	2.99	128	988	2.08	122	0.0268	0.462	--
27	2013-12-16	1.71	2.79	51.5	617	1.72	53.1	-0.00682	-0.174	--
28	2014-01-13	2.15	3.05	140	1120	2.18	152	-0.0307	-0.575	--
29	2014-02-10	2.07	3.01	117	1020	2.1	129	-0.0345	-0.665	--
30	2014-03-10	2.18	3.06	152	1160	2.2	162	-0.0219	-0.434	--
31	2014-04-07	2.1	3	126	991	2.08	123	0.0176	0.25	--
32	2014-05-05	2.03	2.97	107	934	2.04	111	-0.00785	-0.25	--
33	2014-05-19	2.1	3.02	125	1040	2.12	134	-0.0229	-0.462	--
34	2014-06-02	1.78	2.83	60.5	674	1.79	62.1	-0.00478	-0.149	--
35	2014-06-11	1.31	2.61	20.4	404	1.39	25.1	-0.0836	-1.11	--
36	2014-06-30	1.56	2.69	36.4	489	1.54	35.2	0.0211	0.354	--
37	2014-07-14	1.92	2.87	83.5	747	1.87	74.4	0.0565	0.795	--
38	2014-08-11	2.06	2.87	116	738	1.86	72.9	0.208	2.52	--
39	2014-08-25	1.98	2.9	96.3	803	1.92	84.6	0.0625	0.829	--
40	2014-09-08	1.26	2.62	18.2	419	1.42	26.8	-0.161	-1.8	--
41	2014-09-22	1.73	2.75	53.2	558	1.64	44.4	0.085	1.02	--
42	2014-10-06	2.21	3.05	164	1110	2.17	150	0.0449	0.665	--
43	2014-10-20	1.95	2.87	88.9	738	1.86	72.9	0.0927	1.2	--
44	2014-11-17	2.05	2.91	113	817	1.93	87.2	0.119	1.6	--
45	2014-12-15	1.8	2.77	63.1	585	1.68	48.4	0.122	1.69	--
46	2015-01-12	2.12	3	131	997	2.09	124	0.0301	0.518	--
47	2015-02-09	2.17	3.05	147	1130	2.18	155	-0.0163	-0.354	--
48	2015-03-09	2.12	3.02	131	1050	2.12	135	-0.00749	-0.225	--
49	2015-04-06	2.09	2.99	122	972	2.07	119	0.0182	0.302	--
50	2015-05-04	1.84	2.86	68.4	728	1.85	71.1	-0.0107	-0.302	--
51	2015-05-18	1.26	2.53	18.2	337	1.25	18.2	0.0062	0.0744	--
52	2015-06-01	1.37	2.65	23.7	445	1.47	29.8	-0.0928	-1.15	--
53	2015-06-15	1.25	2.57	17.7	369	1.32	21.4	-0.0756	-1.02	--
54	2015-06-29	1.25	2.48	17.7	299	1.16	14.8	0.0852	1.06	--
55	2015-07-13	1.34	2.55	22	354	1.29	19.9	0.0507	0.696	--
56	2015-07-27	1.52	2.73	33	537	1.61	41.5	-0.0934	-1.2	--
57	2015-08-10	1.85	2.87	70.9	741	1.86	73.5	-0.00906	-0.276	--
58	2015-08-24	1.75	2.85	56.7	708	1.82	67.7	-0.0708	-0.939	--
59	2015-09-08	1.89	2.89	77.4	777	1.9	79.8	-0.00707	-0.199	--
60	2015-09-21	1.97	2.93	93.2	860	1.97	95.5	-0.00439	-0.0992	--
61	2015-10-05	1.91	2.91	80.4	808	1.93	85.6	-0.0206	-0.407	--
62	2015-10-19	2.21	3.05	162	1120	2.18	152	0.0327	0.605	--
63	2015-11-16	2.09	2.99	123	982	2.08	121	0.0142	0.199	--
64	2015-12-14	1.53	2.71	33.6	518	1.58	39	-0.0579	-0.795	--
65	2016-01-11	1.51	2.73	32.3	537	1.61	41.5	-0.103	-1.31	--
66	2016-02-08	1.73	2.88	54.3	767	1.89	78	-0.151	-1.69	--
67	2016-03-03	1.9	2.93	80.2	855	1.97	94.6	-0.0652	-0.864	--
68	2016-04-04	2.05	3	113	1010	2.1	127	-0.0443	-0.761	--
69	2016-05-02	1.58	2.8	38.2	626	1.73	54.5	-0.148	-1.6	--
70	2016-05-16	1.36	2.7	23	498	1.55	36.3	-0.192	-2.52	--
71	2016-06-06	1.53	2.7	33.6	496	1.55	36.1	-0.0245	-0.518	--
72	2016-06-20	1.27	2.6	18.8	402	1.39	24.9	-0.115	-1.37	--
73	2016-07-11	1.86	2.89	72.9	777	1.9	79.8	-0.0331	-0.635	--
74	2016-07-25	2.01	2.95	102	887	2	101	0.011	0.174	--
75	2016-08-08	1.68	2.76	47.6	573	1.66	46.6	0.0154	0.225	--

76	2016-08-22	1.89	2.9	77.6	787	1.91	81.7	-0.0158	-0.328	--
77	2016-09-12	1.59	2.72	39.1	523	1.59	39.6	0.000564	0	--
78	2016-09-26	1.94	2.87	86.9	742	1.86	73.6	0.0786	0.978	--
79	2016-10-11	1.9	2.85	80.2	713	1.83	68.6	0.0744	0.901	--
80	2016-10-24	2.17	3.05	148	1110	2.17	150	0.000357	-0.0248	--
81	2016-11-07	2.13	3.04	135	1100	2.16	148	-0.0326	-0.605	--
82	2016-12-12	1.71	2.8	51.2	629	1.73	54.9	-0.0242	-0.489	--
83	2017-01-09	1.95	2.97	89.1	925	2.03	109	-0.0802	-1.06	--
84	2017-02-06	2.09	3.03	122	1080	2.15	143	-0.0625	-0.829	--
85	2017-03-06	2.15	3.04	140	1100	2.16	148	-0.0168	-0.381	--
86	2017-04-10	1.51	2.77	32.6	585	1.68	48.3	-0.164	-1.95	--
87	2017-05-08	1.66	2.76	45.4	573	1.66	46.6	-0.00472	-0.124	--
88	2017-05-22	1.82	2.79	65.5	619	1.72	53.3	0.0955	1.31	--
89	2017-06-05	1.89	2.84	77.6	696	1.81	65.8	0.0783	0.939	--
90	2017-06-19	1.9	2.84	79.5	684	1.8	63.7	0.103	1.51	--
91	2018-10-11	1.23	2.44	17	277	1.1	12.9	0.127	1.8	--
92	2018-11-28	1.5	2.61	31.9	409	1.4	25.7	0.101	1.44	--
93	2018-12-17	1.77	2.74	58.6	553	1.63	43.7	0.133	2.15	--
94	2019-02-05	2.06	3.05	116	1130	2.18	154	-0.117	-1.44	--
95	2019-03-18	1.87	2.87	73.6	749	1.87	74.8	-0.000391	-0.0496	--
96	2019-04-15	2.09	3.09	123	1240	2.25	183	-0.165	-2.15	--
97	2019-05-09	1.28	2.54	19.1	346	1.27	19.1	0.0064	0.0992	--
98	2019-06-25	1.47	2.63	29.2	431	1.44	28.1	0.0224	0.381	--
99	2019-07-15	1.64	2.73	43.4	542	1.62	42.3	0.018	0.276	--
100	2019-08-19	1.69	2.77	48.8	585	1.68	48.3	0.0107	0.149	--
101	2019-09-23	2.13	3.07	134	1190	2.22	169	-0.0935	-1.25	--

Definitions

Cl: Chloride, in milligrams per liter (00940).

Cook's D: Cook's distance (Helsel and others, 2020).

DFFITS: Difference in fits statistic (Helsel and others, 2020).

E.vars: Explanatory variables.

Leverage: An outlier's measure in the x direction (Helsel and others, 2020).

LOESS: Local polynomial regression fitting, or locally estimated scatterplot smoothing (Helsel and others, 2020).

LOWESS: Locally weighted scatterplot smoothing (Cleveland, 1979; Helsel and others, 2020).

MSE: Model standard error (Helsel and others, 2020).

MSPE: Model standard percentage error (Helsel and others, 2020).

Probability(>|t|): The probability that the independent variable has no effect on the dependent variable (Helsel and others, 2020).

RMSE: Root mean square error (Helsel and others, 2020).

SC: Specific conductance, in microsiemens per centimeter at 25 degrees Celsius (00095).

t value: Student's t value; the coefficient divided by its associated standard error (Helsel and others, 2020).

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