

Appendix 2.13. Model Archive Summary for Bicarbonate Concentration at U.S. Geological Survey site 07144100; Little Arkansas River near Sedgwick, Kansas, during September 2012 through December 2019

This model archive summary summarizes the bicarbonate model developed to compute hourly or daily bicarbonate. Model development methods follow U.S. Geological Survey (USGS) guidance from Office of Surface Water/Office of Water Quality Technical Memoranda and USGS Techniques and Methods, book 3, chap. C4 (Rasmussen and others, 2009).

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Site and Model Information

Site Number: 07144100

Site Name: Little Arkansas River near Sedgwick, Kansas

Location: Latitude 37°52'59", longitude 97°25'27" referenced to North American Datum of 1927, in NE 1/4 NW 1/4 NW 1/4 sec.15, T.25 S., R.1 W., Sedgwick County, Kansas; hydrologic unit 11030012.

Equipment: A Sutron Satlink II High Data Rate Collection Platform and a Design Analysis Water Log H350/355 nonsubmersible pressure transducer transfers real-time stage and water-quality data via satellite. The primary reference gage is a Type-A wire-weight gage located on the downstream bridge handrail. Check-bar elevation is 33.614 feet. The orifice is enclosed in a well-screen and attached to a concrete pier on the left downstream side of the bridge. Gage height was measured during September 2012 through December 2019. A YSI 6600 water-quality monitor equipped with water temperature, specific conductance, pH, dissolved oxygen, and turbidity (a YSI Model 6026 [September 1998 through December 2006] and YSI Model 6136 [July 2004 through March 2015]) sensors collected data during April 1998 through March 2015. A YSI EXO2 water-quality monitor equipped with water temperature, specific conductance, pH, dissolved oxygen, turbidity, and fluorescent dissolved organic matter sensors collected data during September 2014 through December 2019. A Hach Nitratax monitor collected nitrate data during March 2012 through December 2019.

Date model was developed: June 1, 2020

Model calibration data period: September 11, 2012 through December 10, 2019

Model Data

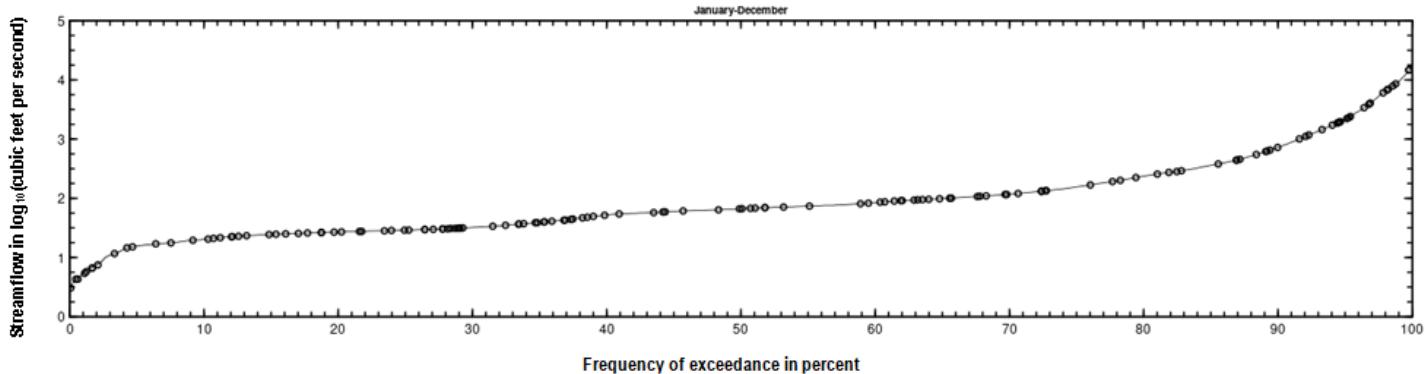
All data were collected using USGS protocols (U.S. Geological Survey, variously dated; Wagner and others, 2006; Sauer and Turnipseed, 2010; Turnipseed and Sauer, 2010) and are stored in the National Water Information System (NWIS) database (U.S. Geological Survey, 2021). Explanatory variables were evaluated individually and in combination. Potential explanatory variables included streamflow, water temperature, specific conductance, pH, dissolved oxygen, YSI EXO2 turbidity, nitrate, and fluorescent dissolved organic matter. Seasonal components (sine and cosine variables) also were evaluated as explanatory variables.

The regression model is based on 135 concomitant values of discretely collected bicarbonate and continuously measured specific conductance during September 2012 through December 2019. Discrete samples were collected over a range of streamflow and specific conductance conditions. No samples had concentrations that were below laboratory detection limits. Summary statistics and the complete model-calibration dataset are provided below. Outliers and influential points were identified using studentized residuals, DFITS, Cook's D (Cook, 1977), and leverage. Outliers in previously published versions of this model (Christensen and others, 2003; Rasmussen and others, 2016) were examined and retained in the dataset if there were no clear issues, explanations, or conditions that would cause a result to be invalid for model calibration. One sample (collection date June 24, 2013) was not representative of the dataset and exceeded Cook's D and DFITS outlier criteria and was removed from the model dataset to avoid erroneous inflation of model-computed values at the upper range of surrogate relations. Removing data points based only on outlier criteria may only overestimate the certainty of the model.

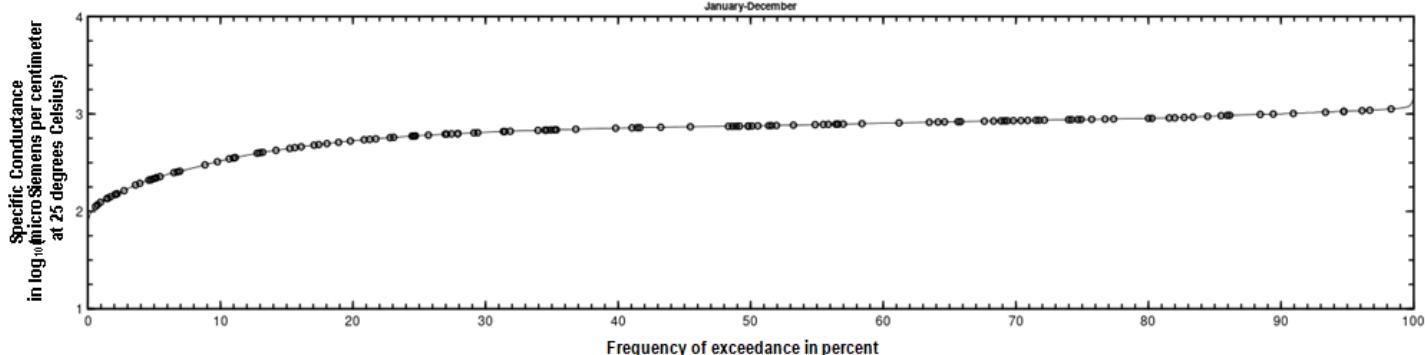
Bicarbonate

Discrete samples were collected from the downstream side of the bridge or instream within 50 feet of the bridge using equal-width-increment, multi-vertical, single vertical or grab-dip methods following U.S. Geological Survey (variously dated) and Rasmussen and others (2014). Discrete samples were collected on a semifixed to event-based schedule ranging from 5 to 22 samples per year with a FISP US DH-95 or D-95 with a Teflon bottle, cap, and nozzle depth-integrating sampler, a DH-81 with a Teflon bottle, cap, and nozzle hand sampler or a grab sample with a Teflon bottle depending on sample location. Samples were analyzed for alkalinity by the U.S. Geological Survey Kansas Water Science Center according to standard methods (Rounds, 2012).

Bicarbonate Samples Plotted on Streamflow Duration Curve



Bicarbonate Samples Plotted on Specific Conductance Duration Curve



Continuous Data

Concomitant specific conductance values were time interpolated. If no concomitant continuous data were available within 2 hours of sample collection, the sample was not included in the dataset.

Model Development

Ordinary least squares regression analysis was done using R (version 4.0.0) programming language (R Core Team, 2020) to relate discretely collected bicarbonate to specific conductance and other continuously measured data. The distribution of residuals was examined for normality and plots of residuals (the difference between the measured and model-calculated values) compared to model-computed bicarbonate were examined for homoscedasticity (departures from zero did not change substantially over the range of model-calculated values). Previously published explanatory variables were also strongly considered for continuity; however, the best explanatory variable(s) was ultimately selected.

Specific conductance was selected as the best predictor of bicarbonate based on residual plots, high coefficient of determination (R^2), and low model standard percentage error (MSPE). Specific conductance was positively related to bicarbonate because it measures water's capacity to conduct an electrical current and is related to the concentration of ionized substances in water (Hem, 1992).

Model Summary

Summary of final bicarbonate regression analysis at USGS site number 07144100:

Bicarbonate-based model:

$$\log_{10}(BC) = 0.984 \times \log_{10}(SC) - 0.409$$

where,

\log_{10} = logarithm base 10;

BC = bicarbonate, in milligrams per liter (mg/L); and

SC = specific conductance, in microsiemens per centimeter at 25 degrees Celsius ($\mu\text{S}/\text{cm}$)

The log-transformed model may be retransformed to original units so that BC 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:

$$BC = 0.3938 \times SC^{0.984}$$

Model Statistics, Data, and Plots

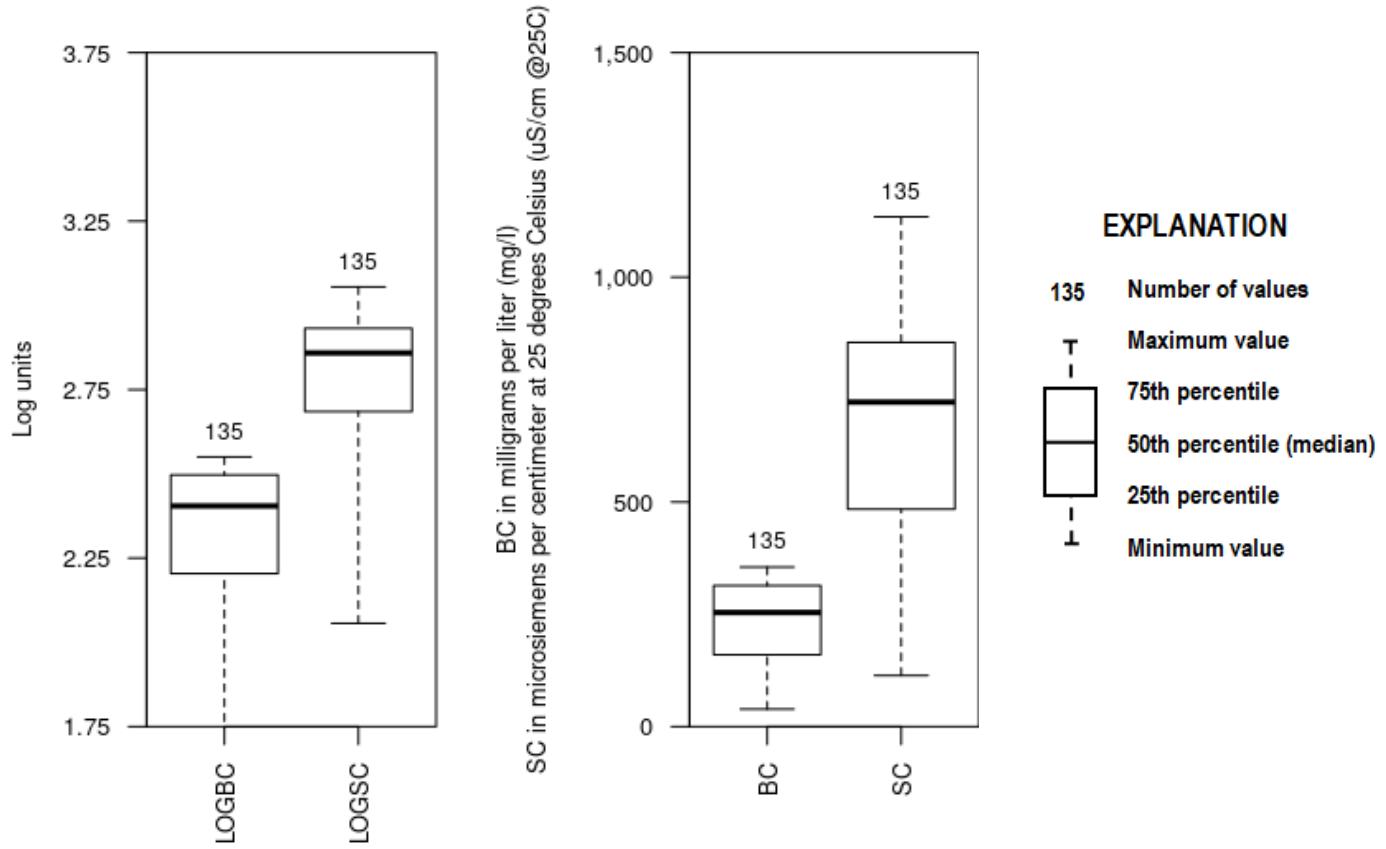
Model

$$\text{LOGBC} = + 0.984 * \text{LOGSC} - 0.409$$

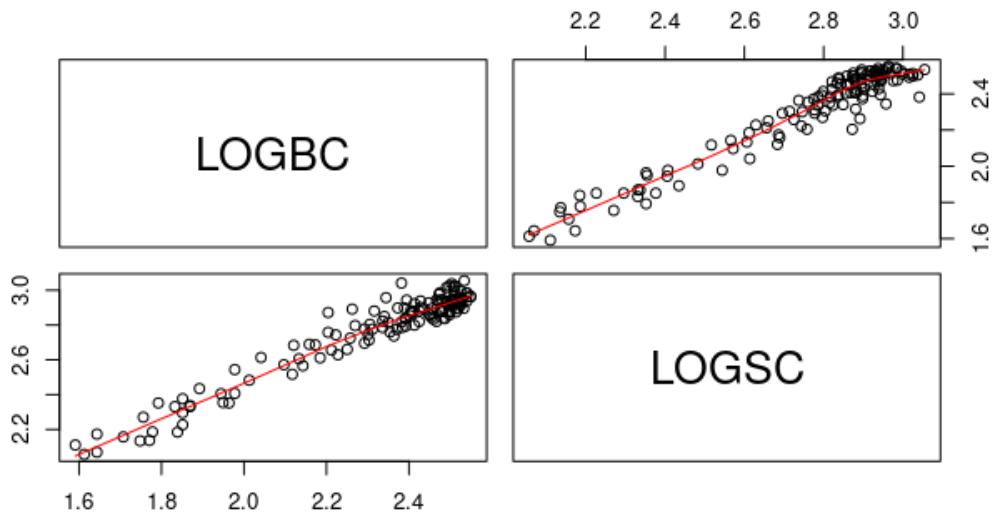
Variable Summary Statistics

	LOGBC	BC	LOGSC	SC
Minimum	1.59	39	2.06	114
1st Quartile	2.20	160	2.68	483
Median	2.40	254	2.86	722
Mean	2.30	230	2.76	651
3rd Quartile	2.50	315	2.93	856
Maximum	2.55	355	3.05	1130

Box Plots



Exploratory Plots



Basic Model Statistics

Number of Observations	135
Standard error (RMSE)	0.0643
Average Model standard percentage error (MSPE)	14.8
Coefficient of determination (R^2)	0.937
Adjusted Coefficient of Determination (Adj. R^2)	0.937
Bias Correction Factor (BCF)	1.01

Explanatory Variables

	Coefficients	Standard Error	t value	Pr(> t)
(Intercept)	-0.409	0.0611	-6.69	5.62e-10
LOGSC	0.984	0.0221	44.60	7.69e-82

Correlation Matrix

	Intercept	E.vars
Intercept	1.000	-0.996
E.vars	-0.996	1.000

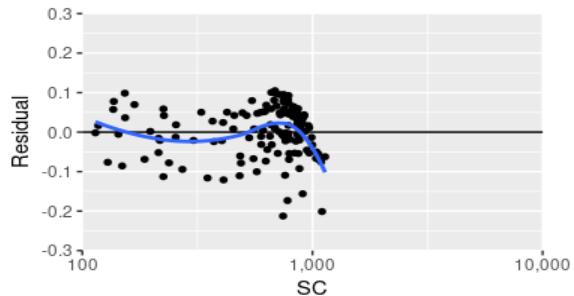
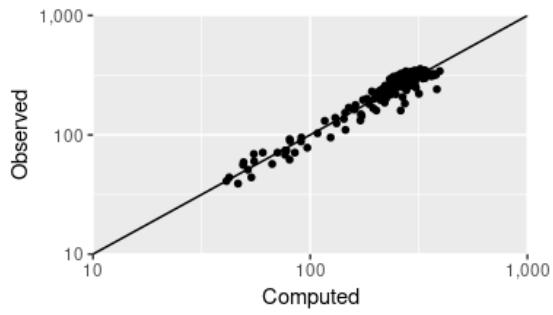
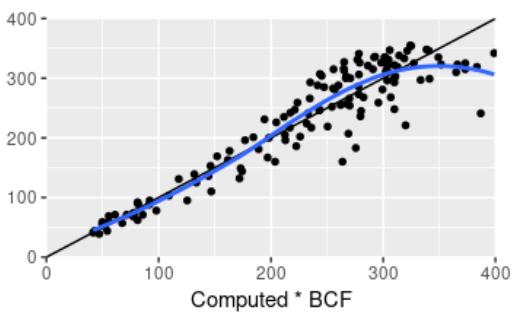
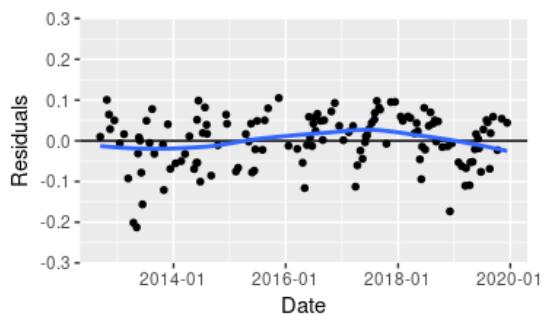
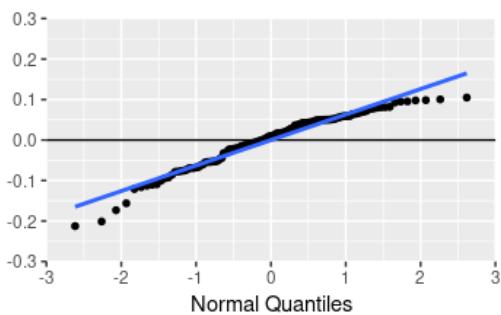
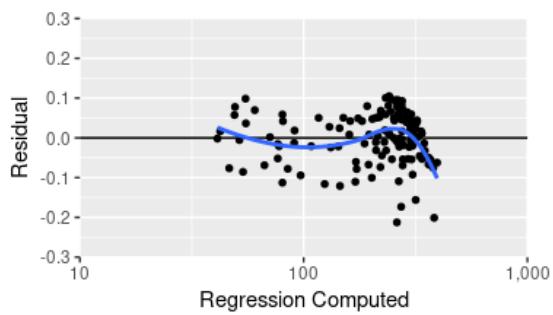
Outlier Test Criteria

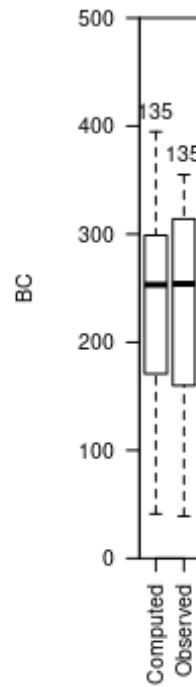
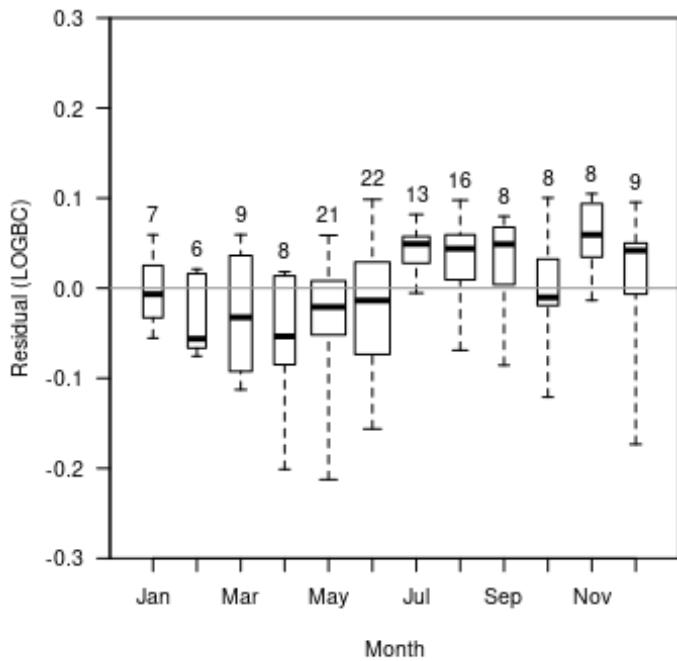
Leverage	Cook's D	DFFITS
0.0444	0.1945	0.2434

Flagged Observations

	LOGBC	Estimate	Residual	Standard Residual	Studentized Residual	Leverage	Cook's D	DFFITS
4/15/2013 9:00	2.38	2.58	-0.201	-3.16	-3.27	0.0169	8.58E-02	-0.429
5/6/2013 11:00	2.2	2.42	-0.213	-3.32	-3.46	0.00896	4.99E-02	-0.329
6/13/2013 9:20	2.34	2.5	-0.156	-2.45	-2.49	0.0121	3.67E-02	-0.276
7/29/2013 10:30	1.71	1.71	-0.0054	-0.0863	-0.086	0.05	1.96E-04	-0.0197
8/15/2013 9:10	1.77	1.69	0.0777	1.24	1.24	0.0529	4.31E-02	0.294
6/12/2014 11:40	1.84	1.74	0.0985	1.57	1.58	0.0461	5.95E-02	0.347
9/3/2014 12:00	1.64	1.73	-0.0856	-1.37	-1.37	0.0477	4.66E-02	-0.306
7/6/2016 11:15	1.75	1.69	0.0574	0.918	0.917	0.0532	2.37E-02	0.217
3/30/2017 13:45	1.79	1.91	-0.113	-1.78	-1.79	0.0268	4.35E-02	-0.298
7/19/2018 11:30	1.78	1.74	0.0364	0.58	0.578	0.0459	8.09E-03	0.127
9/6/2018 12:00	1.61	1.61	-0.00187	-0.03	-0.0299	0.0653	3.15E-05	-0.00791
12/4/2018 11:25	2.26	2.44	-0.173	-2.71	-2.78	0.00953	3.53E-02	-0.273
5/23/2019 12:20	1.64	1.63	0.0165	0.265	0.264	0.0633	2.37E-03	0.0687
6/24/2019 10:40	1.59	1.67	-0.0764	-1.22	-1.23	0.0568	4.51E-02	-0.301

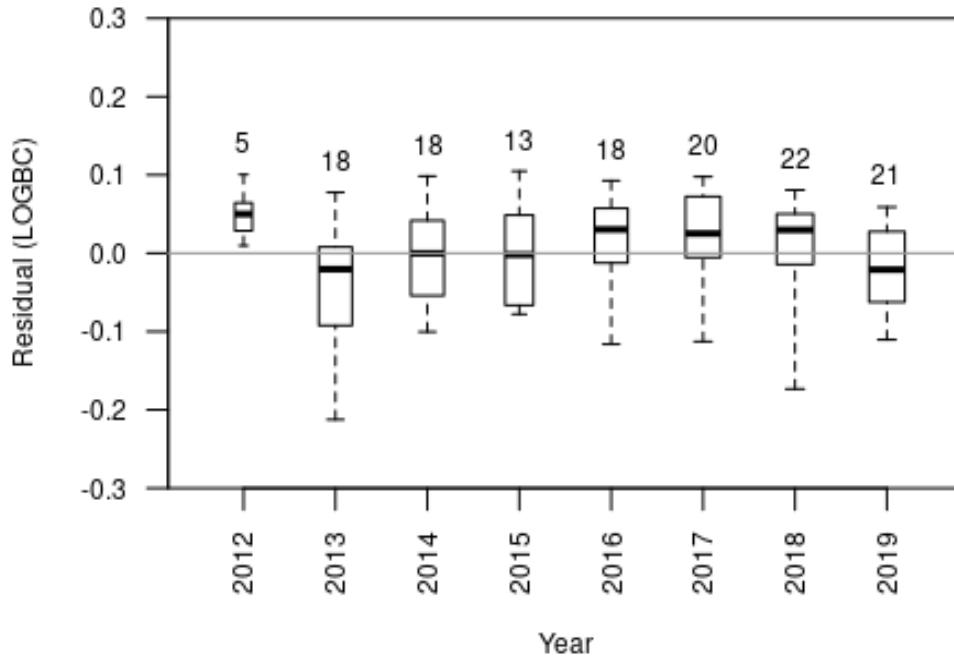
Statistical Plots





EXPLANATION

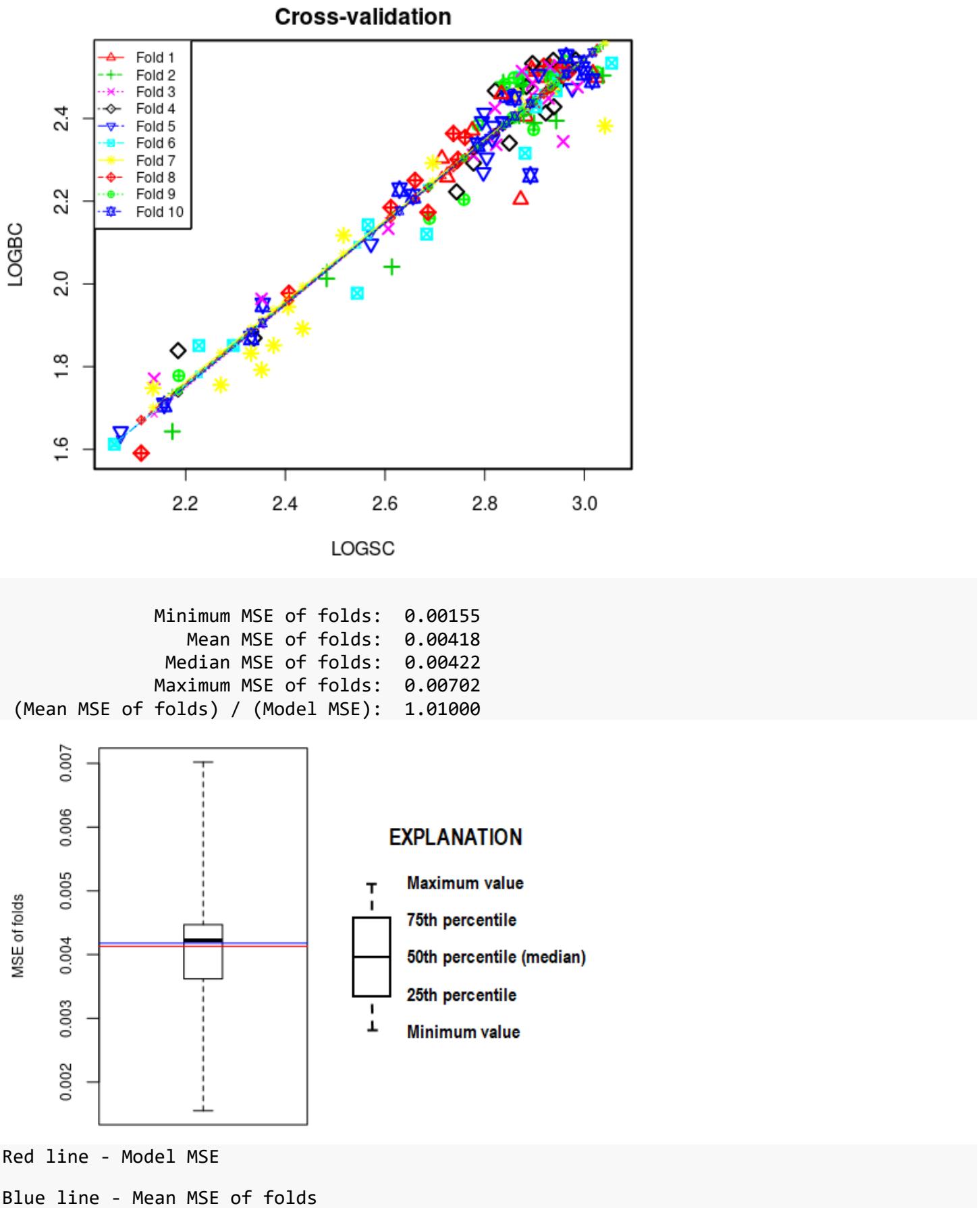
- 135 Number of values
- T Maximum value
- I 75th percentile
- 250 50th percentile (median)
- L 25th percentile
- Minimum value



EXPLANATION

- 5 Number of values
- T Maximum value
- I 75th percentile
- 250 50th percentile (median)
- L 25th percentile
- Minimum value

Cross Validation



Model-Calibration Dataset

	Date	LOGBC	LOGSC	BC	SC	Computed LOGBC	Computed BC	Residual	Normal
									Quantiles
1	9/11/2012	2.39	2.84	246	685	2.38	243	0.00983	0
2	10/24/2012	2.47	2.82	293	663	2.37	235	0.1	2.26
3	11/7/2012	2.53	2.92	335	826	2.46	292	0.0644	1.13
4	11/14/2012	2.51	2.93	321	860	2.48	304	0.0287	0.282
5	12/12/2012	2.53	2.93	335	854	2.48	302	0.05	0.703
6	1/16/2013	2.48	2.94	303	880	2.49	311	-0.00661	-0.224
7	2/13/2013	2.49	2.93	312	860	2.48	304	0.0162	0.0742
8	3/12/2013	2.39	2.94	248	878	2.49	310	-0.0924	-1.37
9	4/15/2013	2.38	3.04	241	1100	2.58	387	-0.201	-2.26
10	5/6/2013	2.2	2.87	160	745	2.42	264	-0.213	-2.62
11	5/15/2013	2.29	2.78	196	599	2.32	213	-0.0313	-0.588
12	5/21/2013	2.21	2.66	163	453	2.2	162	0.00807	-0.0371
13	5/28/2013	2.4	2.86	252	718	2.4	254	0.00041	-0.111
14	6/5/2013	2.16	2.69	144	489	2.24	174	-0.0784	-1.28
15	6/13/2013	2.34	2.96	221	907	2.5	320	-0.156	-1.93
16	7/9/2013	2.45	2.86	283	721	2.4	255	0.0491	0.679
17	7/29/2013	1.71	2.16	51	143	1.71	52.2	-0.0054	-0.186
18	8/15/2013	1.77	2.14	59	137	1.69	49.9	0.0777	1.37
19	8/29/2013	2.34	2.82	217	665	2.37	236	-0.0319	-0.611
20	10/24/2013	2.48	2.94	300	878	2.49	310	-0.00956	-0.263
21	10/30/2013	2.04	2.61	110	411	2.16	147	-0.121	-1.82
22	11/25/2013	2.52	2.94	331	863	2.48	305	0.0403	0.4
23	12/11/2013	2.5	3.03	315	1060	2.57	373	-0.069	-1.06
24	1/14/2014	2.51	3.03	325	1060	2.57	373	-0.0554	-0.88
25	2/20/2014	2.51	3.02	323	1040	2.56	366	-0.05	-0.703
26	3/17/2014	2.51	3	323	998	2.54	352	-0.0324	-0.633
27	4/14/2014	2.54	2.99	346	967	2.53	341	0.011	0.0371
28	5/15/2014	2.37	2.9	236	791	2.44	280	-0.0693	-1.09
29	5/29/2014	2.43	2.94	268	869	2.48	307	-0.0541	-0.853
30	6/3/2014	2.38	2.79	242	612	2.33	217	0.0514	0.827
31	6/5/2014	2.34	2.85	219	707	2.39	250	-0.0539	-0.801
32	6/12/2014	1.84	2.18	69	153	1.74	55.6	0.0985	2.07
33	6/24/2014	2.2	2.76	160	573	2.3	204	-0.1	-1.47
34	7/10/2014	2.38	2.82	241	657	2.36	233	0.0191	0.186
35	7/24/2014	2.52	2.89	331	783	2.44	277	0.0818	1.59
36	8/4/2014	2.5	2.92	315	823	2.46	291	0.0391	0.38
37	8/7/2014	2.46	2.9	286	786	2.44	278	0.0169	0.13
38	9/3/2014	1.64	2.17	44	149	1.73	54.1	-0.0856	-1.32
39	10/16/2014	2.31	2.78	205	598	2.32	212	-0.011	-0.301
40	12/9/2014	2.53	2.92	336	829	2.46	293	0.0642	1.09
41	12/15/2014	2.55	2.96	354	921	2.51	325	0.0417	0.42
42	2/11/2015	2.5	3.04	319	1090	2.58	383	-0.0755	-1.16
43	2/25/2015	2.49	3.02	310	1040	2.56	365	-0.0665	-0.965
44	4/16/2015	2.54	2.98	348	960	2.53	339	0.0164	0.0928
45	5/5/2015	2.42	2.88	266	763	2.43	270	-0.00189	-0.149
46	5/20/2015	1.95	2.35	89	226	1.91	81.7	0.0419	0.44
47	5/27/2015	1.85	2.38	71	238	1.93	85.8	-0.0779	-1.24
48	6/10/2015	2.27	2.8	186	627	2.34	223	-0.0735	-1.13
49	6/17/2015	1.87	2.34	74	217	1.89	78.5	-0.0211	-0.481
50	6/29/2015	2.46	2.87	288	735	2.41	260	0.0487	0.611
51	8/3/2015	2.4	2.88	254	763	2.43	270	-0.0223	-0.524
52	8/17/2015	2.37	2.77	235	596	2.32	212	0.0501	0.727
53	9/8/2015	2.36	2.74	231	546	2.28	194	0.0797	1.42

54	11/17/2015	2.49	2.84	307	687	2.38	244	0.105	2.62
55	1/19/2016	2.41	2.88	257	755	2.42	267	-0.0124	-0.321
56	3/16/2016	2.47	2.94	293	878	2.49	310	-0.02	-0.44
57	4/20/2016	2.39	2.9	245	793	2.44	280	-0.054	-0.827
58	5/3/2016	1.98	2.54	95	350	2.09	125	-0.116	-1.73
59	5/18/2016	2.35	2.82	224	654	2.36	232	-0.0104	-0.282
60	5/31/2016	1.96	2.35	92	225	1.91	81.2	0.0587	0.965
61	6/7/2016	2.3	2.75	200	558	2.29	198	0.00823	-0.0185
62	6/21/2016	1.94	2.41	88	254	1.96	91.6	-0.013	-0.34
63	6/28/2016	2.3	2.71	201	518	2.26	184	0.0421	0.461
64	7/6/2016	1.75	2.13	56	136	1.69	49.6	0.0574	0.936
65	7/13/2016	2.18	2.61	153	409	2.16	146	0.0242	0.243
66	7/25/2016	2.45	2.84	285	698	2.39	247	0.066	1.16
67	8/16/2016	2.29	2.7	196	497	2.24	177	0.049	0.656
68	8/29/2016	1.85	2.3	71	198	1.85	71.4	0.00182	-0.0742
69	9/7/2016	2.23	2.63	169	426	2.18	152	0.0504	0.776
70	10/24/2016	2.51	2.9	326	789	2.44	279	0.072	1.28
71	11/15/2016	2.53	2.9	341	787	2.44	278	0.0927	1.66
72	12/14/2016	2.54	2.96	346	911	2.5	321	0.0365	0.36
73	1/10/2017	2.51	2.97	325	928	2.51	327	0.00138	-0.0928
74	2/14/2017	2.51	2.94	322	878	2.49	310	0.0212	0.205
75	3/14/2017	2.53	2.95	338	890	2.49	314	0.0362	0.321
76	3/30/2017	1.79	2.35	62	225	1.91	81.2	-0.113	-1.66
77	4/11/2017	2.17	2.69	149	485	2.23	173	-0.0604	-0.908
78	5/1/2017	2.1	2.57	125	373	2.12	134	-0.0242	-0.567
79	5/15/2017	2.31	2.8	202	637	2.35	226	-0.0443	-0.656
80	5/31/2017	2.44	2.9	273	786	2.44	278	-0.00357	-0.168
81	6/5/2017	2.39	2.84	247	687	2.38	244	0.0107	0.0185
82	6/13/2017	2.5	2.95	319	886	2.49	313	0.013	0.0556
83	6/28/2017	2.51	2.94	322	862	2.48	304	0.029	0.301
84	7/13/2017	2.45	2.86	281	725	2.41	257	0.0435	0.524
85	7/31/2017	2.39	2.79	247	623	2.34	221	0.0524	0.853
86	8/2/2017	2.41	2.8	259	630	2.35	224	0.0683	1.2
87	8/16/2017	2.48	2.84	304	692	2.39	245	0.0977	1.93
88	8/30/2017	2.5	2.87	316	748	2.42	265	0.0811	1.53
89	9/6/2017	2.5	2.87	313	749	2.42	265	0.0765	1.32
90	10/17/2017	2.41	2.87	255	740	2.41	262	-0.00744	-0.243
91	11/15/2017	2.5	2.86	315	722	2.4	256	0.0949	1.73
92	12/12/2017	2.51	2.87	327	749	2.42	265	0.0954	1.82
93	1/18/2018	2.54	2.94	347	866	2.48	306	0.0594	1.03
94	1/31/2018	2.48	2.88	300	765	2.43	271	0.049	0.633
95	3/6/2018	2.48	2.88	303	754	2.42	267	0.0595	1.06
96	3/22/2018	2.48	2.88	300	753	2.42	267	0.0557	0.908
97	4/18/2018	2.49	2.93	312	856	2.48	302	0.0182	0.149
98	5/2/2018	2.51	2.93	326	844	2.47	298	0.0432	0.502
99	5/9/2018	2.52	2.96	333	904	2.5	319	0.0234	0.224
100	5/23/2018	2.47	2.98	297	945	2.52	333	-0.0457	-0.679
101	6/1/2018	1.89	2.43	78	272	1.99	97.9	-0.0943	-1.42
102	6/6/2018	2.26	2.73	181	531	2.27	189	-0.0143	-0.38
103	6/20/2018	2.46	2.83	288	681	2.38	242	0.0808	1.47
104	6/26/2018	2.13	2.61	136	404	2.16	144	-0.0217	-0.502
105	7/19/2018	1.78	2.19	60	154	1.74	55.8	0.0364	0.34
106	7/31/2018	1.85	2.23	71	168	1.78	61.1	0.0697	1.24
107	8/16/2018	2.25	2.66	178	457	2.21	163	0.0422	0.481
108	8/28/2018	2.12	2.52	131	329	2.07	118	0.0502	0.751
109	9/6/2018	1.61	2.06	41	114	1.61	41.6	-0.00187	-0.13

110	9/18/2018	2.35	2.76	226	576	2.31	205	0.0474	0.588
111	10/16/2018	1.87	2.33	74	215	1.88	77.5	-0.0155	-0.4
112	11/19/2018	2.53	3	335	991	2.54	349	-0.0135	-0.36
113	12/4/2018	2.26	2.89	183	779	2.44	276	-0.173	-2.07
114	12/17/2018	2.47	2.93	296	859	2.48	304	-0.00645	-0.205
115	1/29/2019	2.41	2.92	259	837	2.47	296	-0.0531	-0.776
116	2/19/2019	2.53	3.05	342	1130	2.6	399	-0.0623	-0.936
117	3/14/2019	2.12	2.68	132	483	2.23	172	-0.11	-1.59
118	3/19/2019	2.22	2.74	167	554	2.29	197	-0.0674	-0.995
119	4/11/2019	2.32	2.88	207	760	2.43	269	-0.109	-1.53
120	4/16/2019	2.48	2.99	299	968	2.53	341	-0.053	-0.751
121	5/1/2019	1.83	2.33	68	214	1.88	77.4	-0.0519	-0.727
122	5/15/2019	2.01	2.48	103	304	2.03	109	-0.0209	-0.461
123	5/23/2019	1.64	2.07	44	117	1.63	42.8	0.0165	0.111
124	6/5/2019	2.34	2.79	217	610	2.33	217	0.00486	-0.0556
125	6/12/2019	2.43	2.9	268	799	2.45	282	-0.0183	-0.42
126	6/24/2019	1.59	2.11	39	129	1.67	47	-0.0764	-1.2
127	7/10/2019	2.14	2.57	139	368	2.12	132	0.0277	0.263
128	7/30/2019	2.53	2.93	335	853	2.47	301	0.0506	0.801
129	8/7/2019	2.49	2.9	306	787	2.44	278	0.0455	0.567
130	8/20/2019	1.76	2.27	57	186	1.82	67.5	-0.0689	-1.03
131	8/26/2019	1.98	2.41	95	255	1.96	92	0.0185	0.168
132	9/11/2019	2.42	2.82	266	662	2.37	235	0.059	0.995
133	10/9/2019	2.45	2.93	281	847	2.47	299	-0.023	-0.545
134	11/6/2019	2.51	2.91	321	810	2.45	286	0.0541	0.88
135	12/11/2019	2.55	2.96	355	919	2.51	324	0.044	0.545

Definitions

BC: Bicarbonate in mg/L (00453)

SC: Specific conductance in $\mu\text{S}/\text{cm}$ @25C (00095)

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