Appendix 2.11. Model Archive Summary for Alkalinity 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 alkalinity model developed to compute hourly or daily alkalinity. 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 11, 2019

Model Data

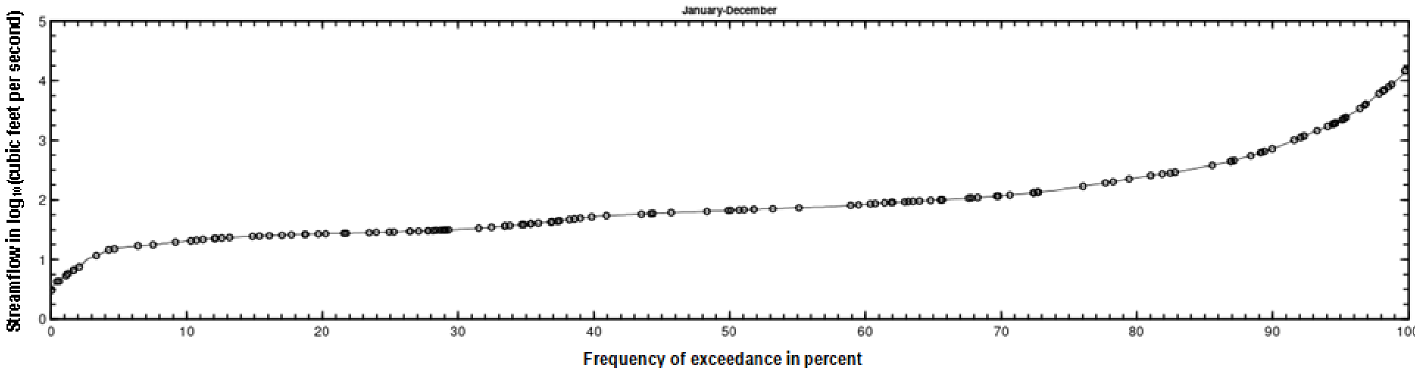
All data were collected using USGS protocols (U.S. Geological Survey, variously dated; Wagner and others, 2006; Sauer and Turnipseed, 2010; Turnipseed and Sauer, 2010) and are stored in the National Water Information System (NWIS) database (U.S. Geological Survey, 2021). Explanatory variables were evaluated 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 alkalinity 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.

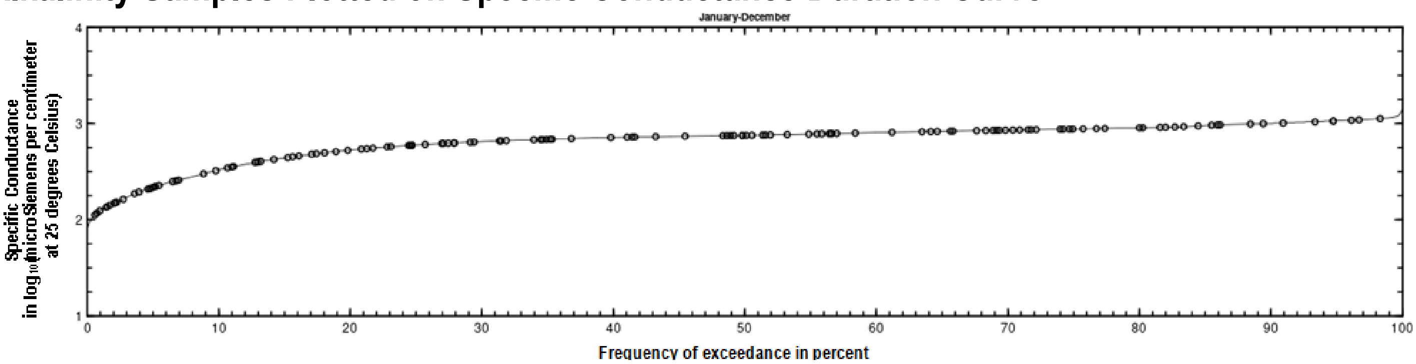
Alkalinity

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 6 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).

Alkalinity Samples Plotted on Streamflow Duration Curve



Alkalinity 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 alkalinity 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 alkalinity 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 alkalinity based on residual plots, high coefficient of determination (R^2), and low model standard percentage error (MSPE). Specific conductance was positively related to total alkalinity 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 alkalinity regression analysis at USGS site number 07144100:

Alkalinity-based model:

$$\log_{10}(ALK) = 0.988 \times \log_{10}(SC) - 0.503$$

where,

$\log_{10}$ = logarithm base 10;
ALK = alkalinity, in milligrams per liter as calcium carbonate (mg/L as $CaCO_3$); and
SC = specific conductance, in microsiemens per centimeter at 25 degrees Celsius (µS/cm)

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

$$ALK = 0.3172 \times SC^{0.988}$$

Model Statistics, Data, and Plots

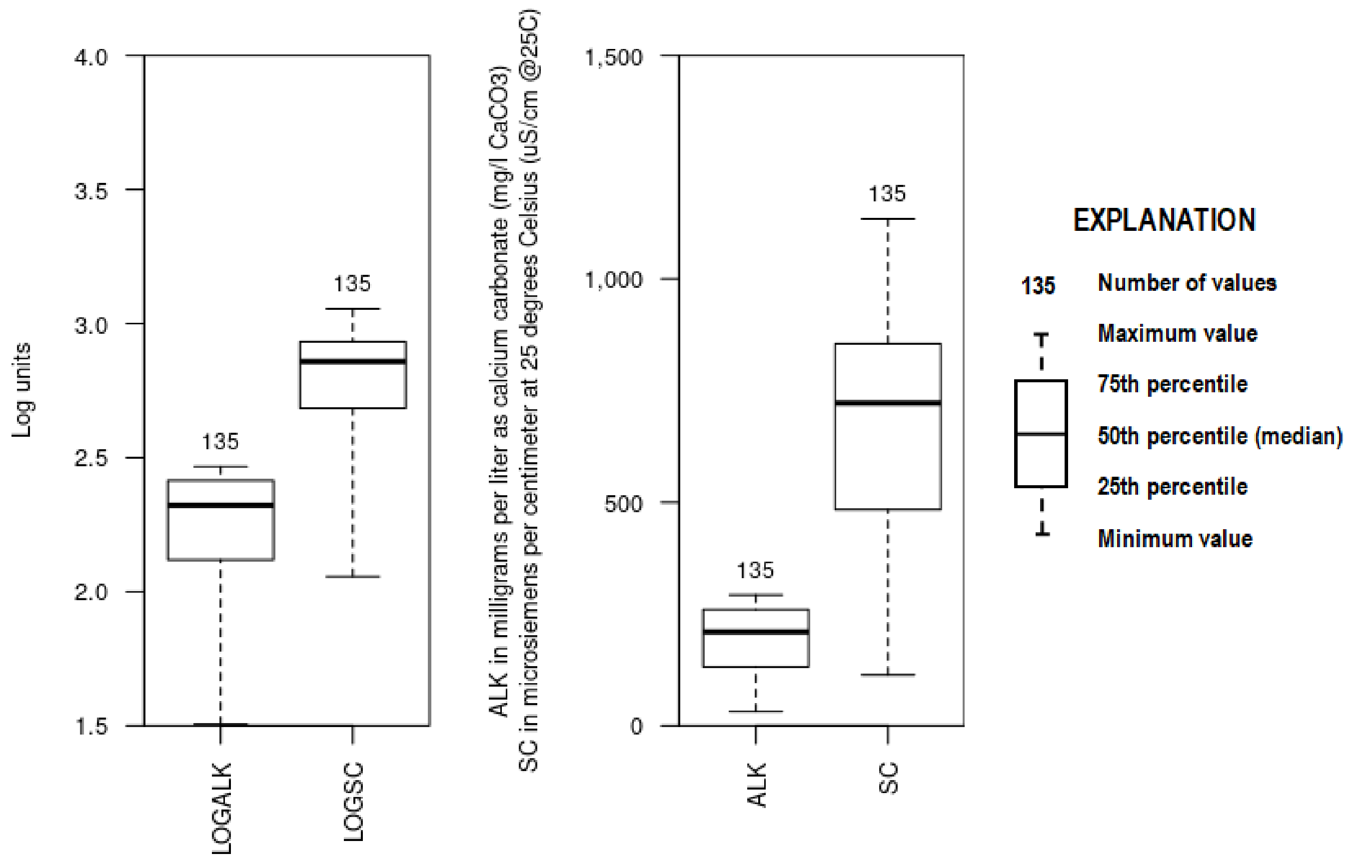
Model

LOGALK = + 0.988 * LOGSC - 0.503

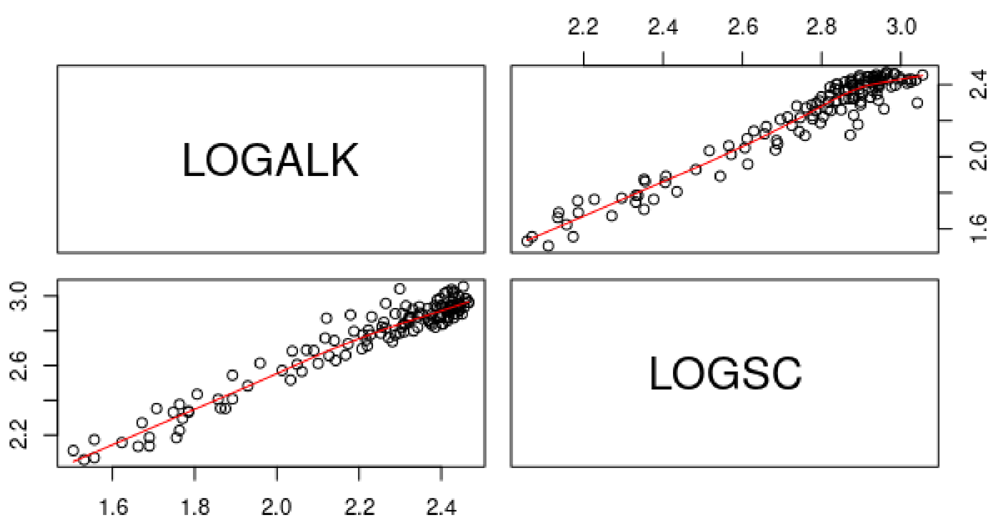
Variable Summary Statistics

```
               LOGALK ALK LOGSC   SC
Minimum          1.51  32  2.06  114
1st Quartile     2.12 131  2.68  483
Median           2.32 210  2.86  722
Mean             2.22 190  2.76  651
3rd Quartile     2.41 260  2.93  856
Maximum          2.47 293  3.05 1130
```

Box Plots



Exploratory Plots



Basic Model Statistics

Number of Observations	135
Standard error (RMSE)	0.0644
Average Model standard percentage error (MSPE)	14.9
Coefficient of determination (R^2)	0.938
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)	-0.503	0.0612	-8.22	1.61e-13
LOGSC	0.988	0.0221	44.70	5.94e-82

Correlation Matrix

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

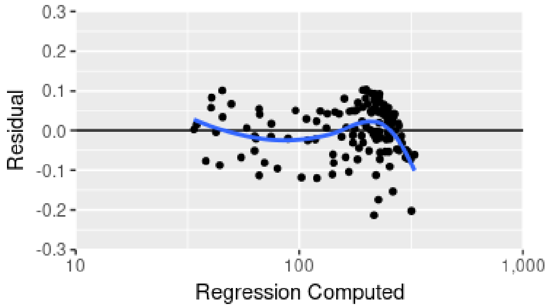
Outlier Test Criteria

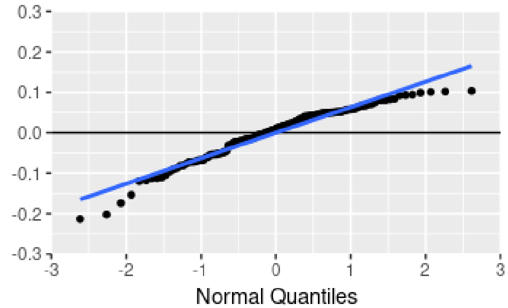
Leverage	Cook's D	DFFITS
0.0444	0.1945	0.2434

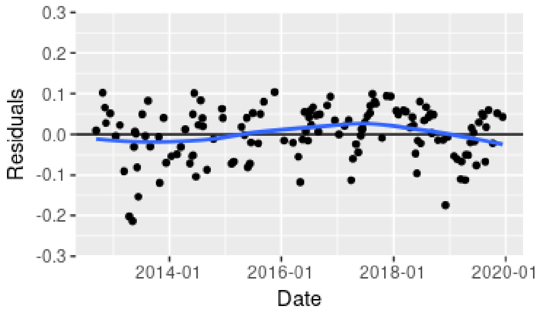
Flagged Observations

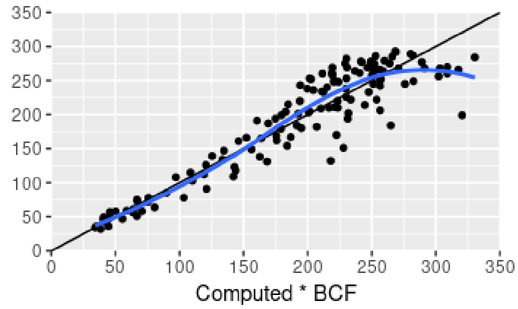
	LOGALK	Estimate	Residual	Standard Residual	Studentized Residual	Leverage	Cook's D	DFFITS
4/15/2013 9:00	2.3	2.5	-0.202	-3.17	-3.29	0.0169	8.65E-02	-0.431
5/6/2013 11:00	2.12	2.33	-0.213	-3.33	-3.47	0.00896	5.02E-02	-0.33
6/13/2013 9:20	2.26	2.42	-0.154	-2.4	-2.44	0.0121	3.53E-02	-0.271
7/29/2013 10:30	1.62	1.63	-0.00417	-0.0665	-0.0662	0.05	1.16E-04	-0.0152
8/15/2013 9:10	1.69	1.61	0.0827	1.32	1.32	0.0529	4.86E-02	0.313
6/12/2014 11:40	1.76	1.65	0.101	1.61	1.61	0.0461	6.23E-02	0.355
9/3/2014 12:00	1.56	1.64	-0.0873	-1.39	-1.39	0.0477	4.83E-02	-0.312
7/6/2016 11:15	1.66	1.61	0.0576	0.919	0.918	0.0532	2.37E-02	0.218
3/30/2017 13:45	1.71	1.82	-0.113	-1.78	-1.79	0.0268	4.34E-02	-0.297
7/19/2018 11:30	1.69	1.66	0.0339	0.539	0.537	0.0459	6.98E-03	0.118
9/6/2018 12:00	1.53	1.53	0.00279	0.0449	0.0447	0.0653	7.03E-05	0.0118
12/4/2018 11:25	2.18	2.35	-0.174	-2.72	-2.79	0.00953	3.56E-02	-0.274
5/23/2019 12:20	1.56	1.54	0.0153	0.245	0.244	0.0633	2.02E-03	0.0634
6/24/2019 10:40	1.51	1.58	-0.0766	-1.22	-1.23	0.0568	4.51E-02	-0.301

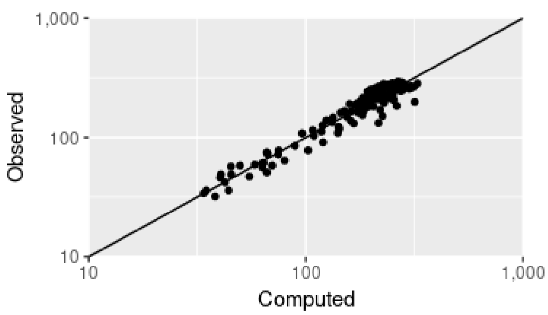
Statistical Plots

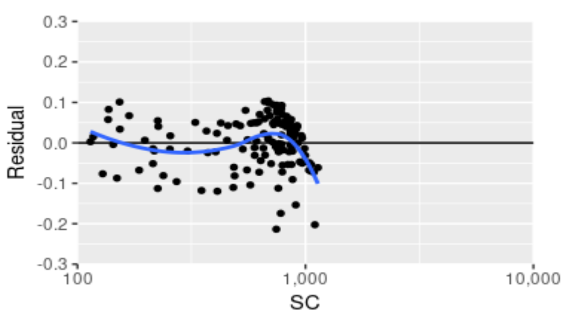


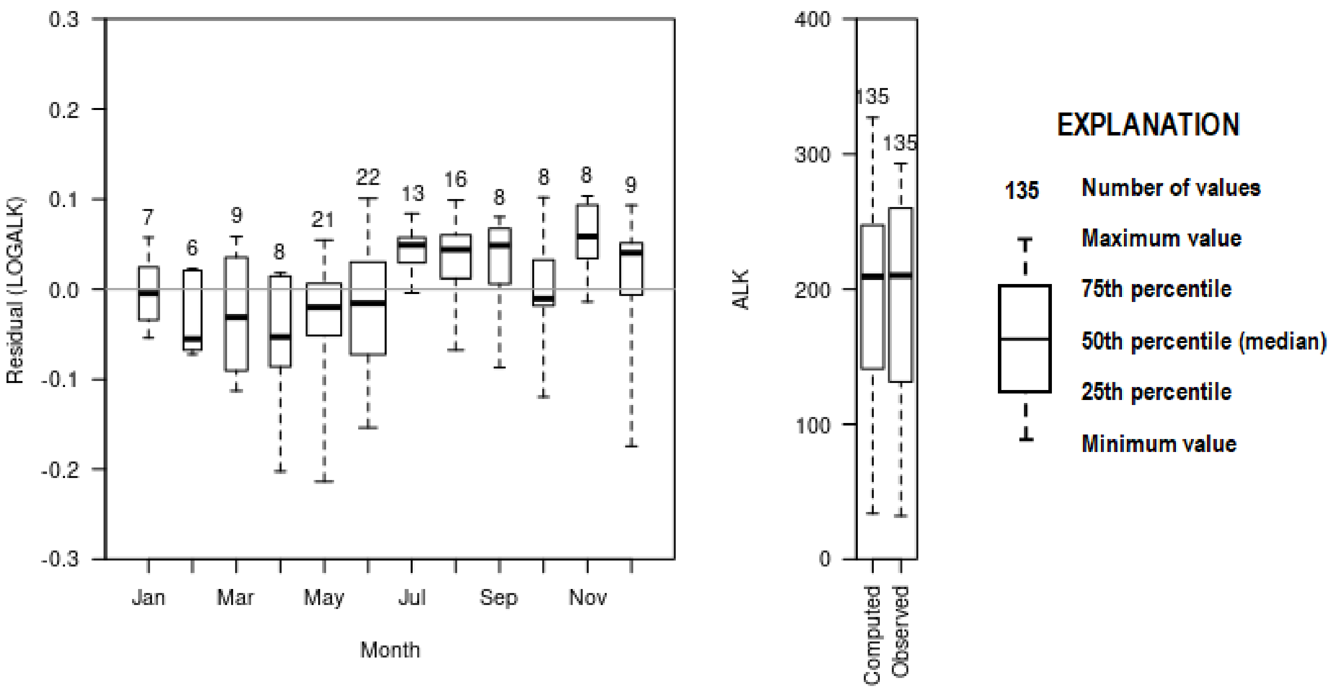


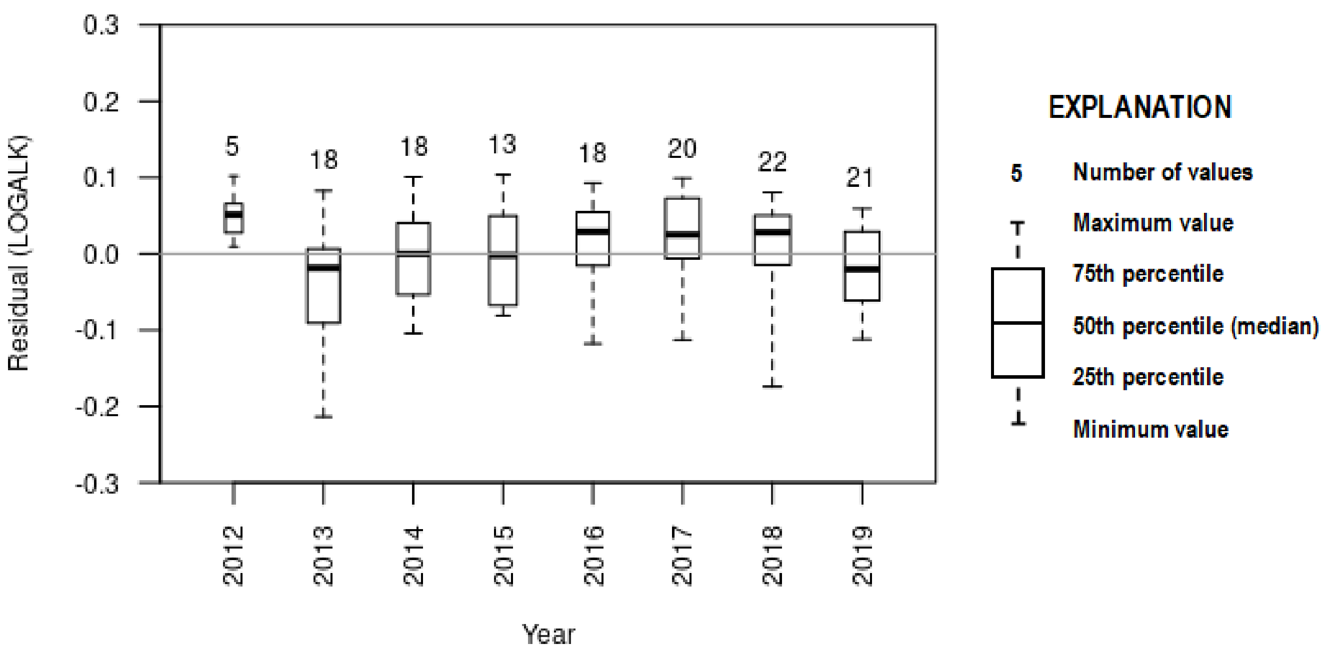




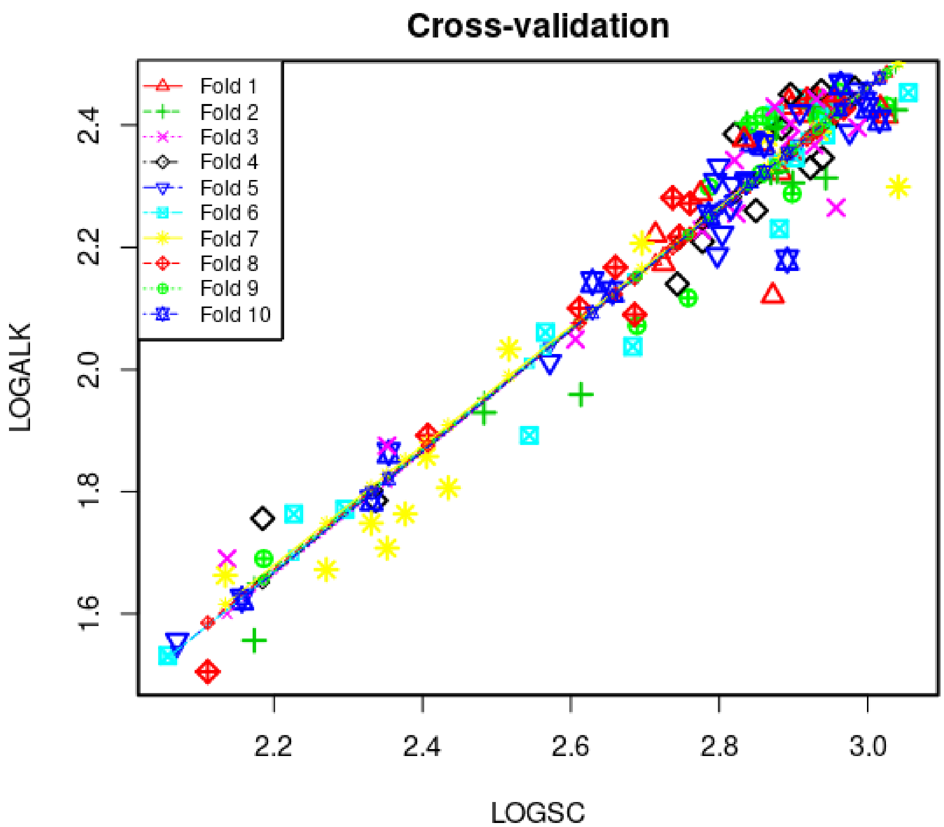





0.3
0.2
0.1
0.0
-0.1
-0.2
-0.3
Residual (LOGALK)
7
6
9
8
21
22
13
16
8
8
8
9
Jan
Mar
May
Jul
Sep
Nov
Month
400
300
200
100
0
ALK
135
135
Computed
Observed
EXPLANATION
135
Number of values
Maximum value
75th percentile
50th percentile (median)
25th percentile
Minimum value


0.3
0.2
0.1
0.0
-0.1
-0.2
-0.3
Residual (LOGALK)
5
18
18
13
18
20
22
21
2012
2013
2014
2015
2016
2017
2018
2019
Year
EXPLANATION
5
Number of values
Maximum value
75th percentile
50th percentile (median)
25th percentile
Minimum value

Cross Validation

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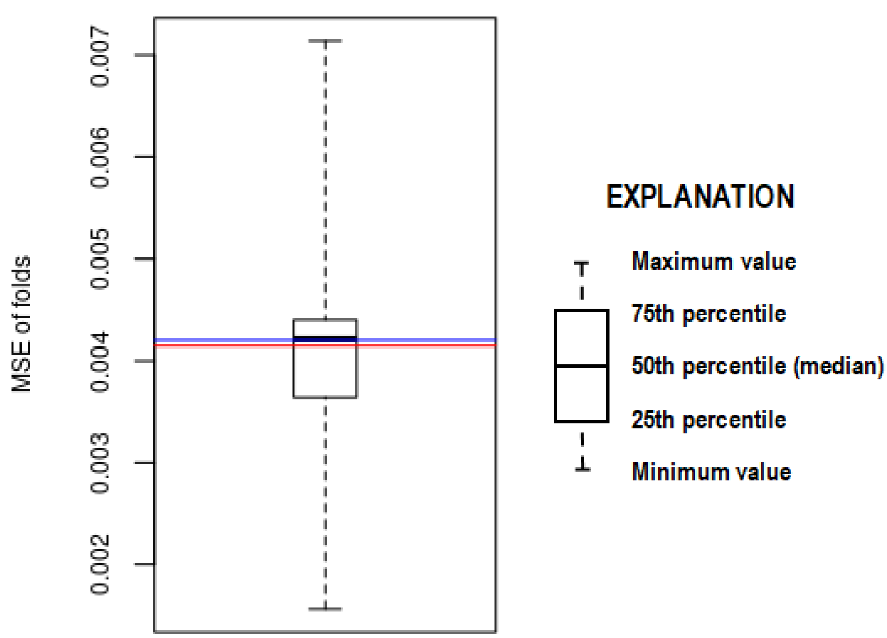
               Minimum MSE of folds:  0.00156
                  Mean MSE of folds:  0.00420
                Median MSE of folds:  0.00421
               Maximum MSE of folds:  0.00714
 (Mean MSE of folds) / (Model MSE):  1.01000
```

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Red line - Model MSE

Blue line - Mean MSE of folds
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Model-Calibration Dataset

	Date	LOGALK	LOGSC	ALK	SC	Computed LOGALK	Computed ALK	Residual	Normal Quantiles
1	9/11/2012	2.31	2.84	203	685	2.3	201	0.00914	0
2	10/24/2012	2.39	2.82	243	663	2.28	194	0.102	2.26
3	11/7/2012	2.44	2.92	278	826	2.38	241	0.0658	1.13
4	11/14/2012	2.42	2.93	265	860	2.4	251	0.0278	0.263
5	12/12/2012	2.44	2.93	278	854	2.39	250	0.0514	0.801
6	1/16/2013	2.4	2.94	252	880	2.41	257	-0.00436	-0.205
7	2/13/2013	2.42	2.93	262	860	2.4	251	0.0227	0.205
8	3/12/2013	2.31	2.94	206	878	2.4	256	-0.0907	-1.37
9	4/15/2013	2.3	3.04	199	1100	2.5	320	-0.202	-2.26
10	5/6/2013	2.12	2.87	132	745	2.33	218	-0.213	-2.62
11	5/15/2013	2.21	2.78	162	599	2.24	176	-0.0311	-0.611
12	5/21/2013	2.13	2.66	134	453	2.12	133	0.00648	-0.0371
13	5/28/2013	2.32	2.86	209	718	2.32	210	0.00182	-0.111
14	6/5/2013	2.07	2.69	118	489	2.15	144	-0.0815	-1.28
15	6/13/2013	2.26	2.96	184	907	2.42	265	-0.154	-1.93
16	7/9/2013	2.37	2.86	234	721	2.32	211	0.0492	0.679
17	7/29/2013	1.62	2.16	42	143	1.63	42.8	-0.00417	-0.186
18	8/15/2013	1.69	2.14	49	137	1.61	40.9	0.0827	1.53
19	8/29/2013	2.26	2.82	180	665	2.29	195	-0.0303	-0.588
20	10/24/2013	2.4	2.94	250	878	2.4	256	-0.00644	-0.243
21	10/30/2013	1.96	2.61	91	411	2.08	121	-0.12	-1.82
22	11/25/2013	2.44	2.94	274	863	2.4	252	0.0406	0.44
23	12/11/2013	2.41	3.03	260	1060	2.49	309	-0.0704	-1.06
24	1/14/2014	2.43	3.03	270	1060	2.49	309	-0.054	-0.853
25	2/20/2014	2.43	3.02	268	1040	2.48	303	-0.0491	-0.703
26	3/17/2014	2.43	3	268	998	2.46	291	-0.0314	-0.633
27	4/14/2014	2.46	2.99	287	967	2.45	282	0.0119	0.0185
28	5/15/2014	2.29	2.9	194	791	2.36	231	-0.072	-1.09
29	5/29/2014	2.35	2.94	222	869	2.4	254	-0.0536	-0.801
30	6/3/2014	2.3	2.79	199	612	2.25	179	0.0494	0.703
31	6/5/2014	2.26	2.85	182	707	2.31	207	-0.0515	-0.776
32	6/12/2014	1.76	2.18	57	153	1.65	45.7	0.101	2.07
33	6/24/2014	2.12	2.76	131	573	2.22	168	-0.104	-1.47
34	7/10/2014	2.3	2.82	201	657	2.28	193	0.0231	0.224
35	7/24/2014	2.44	2.89	275	783	2.36	229	0.0838	1.59
36	8/4/2014	2.42	2.92	261	823	2.38	241	0.0399	0.38
37	8/7/2014	2.38	2.9	238	786	2.36	230	0.0196	0.149
38	9/3/2014	1.56	2.17	36	149	1.64	44.5	-0.0873	-1.32
39	10/16/2014	2.23	2.78	169	598	2.24	176	-0.0119	-0.282
40	12/9/2014	2.44	2.92	277	829	2.38	242	0.0627	1.09
41	12/15/2014	2.47	2.96	292	921	2.43	269	0.0403	0.4
42	2/11/2015	2.42	3.04	266	1090	2.5	318	-0.0725	-1.13
43	2/25/2015	2.41	3.02	256	1040	2.48	302	-0.0676	-0.995
44	4/16/2015	2.46	2.98	289	960	2.44	280	0.0179	0.13
45	5/5/2015	2.34	2.88	220	763	2.34	223	-0.00179	-0.149
46	5/20/2015	1.86	2.35	73	226	1.82	67.2	0.0406	0.42
47	5/27/2015	1.76	2.38	58	238	1.84	70.6	-0.0811	-1.24
48	6/10/2015	2.19	2.8	154	627	2.26	184	-0.0726	-1.16
49	6/17/2015	1.79	2.34	61	217	1.81	64.6	-0.0202	-0.461
50	6/29/2015	2.38	2.87	240	735	2.33	215	0.0521	0.853
51	8/3/2015	2.32	2.88	210	763	2.34	223	-0.0224	-0.545
52	8/17/2015	2.29	2.77	194	596	2.24	175	0.0498	0.727
53	9/8/2015	2.28	2.74	191	546	2.2	160	0.0803	1.37

54	11/17/2015	2.4	2.84	253	687	2.3	201	0.104	2.62
55	1/19/2016	2.32	2.88	211	755	2.34	221	-0.0155	-0.36
56	3/16/2016	2.38	2.94	242	878	2.4	256	-0.0207	-0.481
57	4/20/2016	2.31	2.9	202	793	2.36	232	-0.0553	-0.88
58	5/3/2016	1.89	2.54	78	350	2.01	103	-0.118	-1.73
59	5/18/2016	2.26	2.82	184	654	2.28	192	-0.013	-0.301
60	5/31/2016	1.88	2.35	75	225	1.82	66.8	0.0547	0.908
61	6/7/2016	2.22	2.75	165	558	2.21	164	0.00781	-0.0185
62	6/21/2016	1.86	2.41	72	254	1.87	75.4	-0.0156	-0.4
63	6/28/2016	2.22	2.71	166	518	2.18	152	0.0422	0.481
64	7/6/2016	1.66	2.13	46	136	1.61	40.7	0.0576	0.965
65	7/13/2016	2.1	2.61	126	409	2.08	121	0.0236	0.243
66	7/25/2016	2.37	2.84	236	698	2.31	204	0.0668	1.16
67	8/16/2016	2.21	2.7	161	497	2.16	146	0.0469	0.588
68	8/29/2016	1.77	2.3	59	198	1.76	58.7	0.00639	-0.0556
69	9/7/2016	2.14	2.63	139	426	2.09	125	0.0491	0.656
70	10/24/2016	2.43	2.9	269	789	2.36	231	0.0711	1.28
71	11/15/2016	2.45	2.9	282	787	2.36	230	0.0927	1.66
72	12/14/2016	2.45	2.96	285	911	2.42	266	0.0345	0.34
73	1/10/2017	2.43	2.97	268	928	2.43	271	-0.000165	-0.13
74	2/14/2017	2.42	2.94	266	878	2.4	256	0.0205	0.168
75	3/14/2017	2.45	2.95	279	890	2.41	260	0.0352	0.36
76	3/30/2017	1.71	2.35	51	225	1.82	66.8	-0.113	-1.66
77	4/11/2017	2.09	2.69	123	485	2.15	143	-0.0603	-0.908
78	5/1/2017	2.01	2.57	103	373	2.04	110	-0.0244	-0.567
79	5/15/2017	2.22	2.8	167	637	2.27	187	-0.044	-0.656
80	5/31/2017	2.35	2.9	226	786	2.36	230	-0.00312	-0.168
81	6/5/2017	2.31	2.84	205	687	2.3	201	0.0125	0.0371
82	6/13/2017	2.42	2.95	264	886	2.41	259	0.0131	0.0556
83	6/28/2017	2.43	2.94	267	862	2.4	252	0.03	0.301
84	7/13/2017	2.37	2.86	233	725	2.32	212	0.0448	0.545
85	7/31/2017	2.31	2.79	204	623	2.26	183	0.0523	0.88
86	8/2/2017	2.33	2.8	215	630	2.26	185	0.0703	1.24
87	8/16/2017	2.4	2.84	252	692	2.3	203	0.099	1.93
88	8/30/2017	2.42	2.87	261	748	2.34	219	0.0807	1.42
89	9/6/2017	2.41	2.87	258	749	2.34	219	0.0752	1.32
90	10/17/2017	2.32	2.87	210	740	2.33	217	-0.00915	-0.263
91	11/15/2017	2.41	2.86	260	722	2.32	211	0.0943	1.82
92	12/12/2017	2.43	2.87	269	749	2.34	219	0.0932	1.73
93	1/18/2018	2.46	2.94	286	866	2.4	253	0.0577	0.995
94	1/31/2018	2.39	2.88	248	765	2.35	224	0.0488	0.633
95	3/6/2018	2.4	2.88	250	754	2.34	221	0.0585	1.03
96	3/22/2018	2.39	2.88	248	753	2.34	220	0.0556	0.936
97	4/18/2018	2.41	2.93	257	856	2.39	250	0.0163	0.0928
98	5/2/2018	2.43	2.93	269	844	2.39	247	0.0422	0.461
99	5/9/2018	2.44	2.96	275	904	2.42	264	0.0225	0.186
100	5/23/2018	2.39	2.98	245	945	2.44	276	-0.0471	-0.679
101	6/1/2018	1.81	2.43	64	272	1.9	80.6	-0.0959	-1.42
102	6/6/2018	2.17	2.73	149	531	2.19	156	-0.0156	-0.38
103	6/20/2018	2.38	2.83	238	681	2.3	200	0.0807	1.47
104	6/26/2018	2.05	2.61	112	404	2.07	119	-0.0223	-0.524
105	7/19/2018	1.69	2.19	49	154	1.66	45.8	0.0339	0.321
106	7/31/2018	1.76	2.23	58	168	1.7	50.2	0.0671	1.2
107	8/16/2018	2.17	2.66	147	457	2.12	135	0.0426	0.502
108	8/28/2018	2.03	2.52	108	329	1.98	97.2	0.0505	0.776
109	9/6/2018	1.53	2.06	34	114	1.53	34.1	0.00279	-0.0928

110	9/18/2018	2.27	2.76	187	576	2.22	169	0.0482	0.611
111	10/16/2018	1.79	2.33	61	215	1.8	63.7	-0.0146	-0.34
112	11/19/2018	2.44	3	277	991	2.46	289	-0.014	-0.321
113	12/4/2018	2.18	2.89	151	779	2.35	228	-0.174	-2.07
114	12/17/2018	2.39	2.93	245	859	2.4	251	-0.00624	-0.224
115	1/29/2019	2.33	2.92	214	837	2.38	245	-0.0536	-0.827
116	2/19/2019	2.45	3.05	284	1130	2.51	330	-0.0612	-0.936
117	3/14/2019	2.04	2.68	109	483	2.15	142	-0.11	-1.53
118	3/19/2019	2.14	2.74	138	554	2.21	163	-0.0671	-0.965
119	4/11/2019	2.23	2.88	170	760	2.34	222	-0.112	-1.59
120	4/16/2019	2.4	2.99	249	968	2.45	283	-0.0504	-0.727
121	5/1/2019	1.75	2.33	56	214	1.8	63.7	-0.0514	-0.751
122	5/15/2019	1.93	2.48	85	304	1.95	90	-0.0201	-0.44
123	5/23/2019	1.56	2.07	36	117	1.54	35.1	0.0153	0.0742
124	6/5/2019	2.25	2.79	179	610	2.25	179	0.00421	-0.0742
125	6/12/2019	2.35	2.9	222	799	2.36	234	-0.0176	-0.42
126	6/24/2019	1.51	2.11	32	129	1.58	38.6	-0.0766	-1.2
127	7/10/2019	2.06	2.57	115	368	2.03	109	0.0292	0.282
128	7/30/2019	2.44	2.93	277	853	2.39	249	0.0504	0.751
129	8/7/2019	2.4	2.9	253	787	2.36	230	0.0454	0.567
130	8/20/2019	1.67	2.27	47	186	1.74	55.5	-0.0676	-1.03
131	8/26/2019	1.89	2.41	78	255	1.87	75.7	0.0174	0.111
132	9/11/2019	2.34	2.82	220	662	2.28	194	0.0593	1.06
133	10/9/2019	2.37	2.93	233	847	2.39	248	-0.022	-0.502
134	11/6/2019	2.42	2.91	264	810	2.37	237	0.0517	0.827
135	12/11/2019	2.47	2.96	293	919	2.42	268	0.0429	0.524

Definitions

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ALK: Alkalinity in mg/L CaCO3 (39086)
SC: Specific conductance in µS/cm @25C (00095)
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