

Appendix 6.1. Model Archive Summary for Bromide Concentration at U.S. Geological Survey station 375350097262800; Little Arkansas River upstream of ASR Facility near Sedgwick, Kansas, during April 2011 through October 2021

This model archive summary summarizes the bromide model developed to compute hourly or daily bromide. 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: 375350097262800

Site Name: Little Arkansas River upstream of ASR Facility near Sedgwick, Kansas

Location: Latitude 37°53'49.7", longitude 97°26'28.0" referenced to North American Datum of 1983, in NE 1/4 NW 1/4 NW 1/4 sec.9, T.25 S., R.1 W., Sedgwick County, Kansas; hydrologic unit 11030012.

Equipment: A Sutron Satlink II High Data Rate Collection Platform (DCP) collected and transmitted stage data measured by a Sutron submersible pressure transducer and water-quality data measured by a water-quality and nitrate monitors. The DCP transmitted real-time stage and water-quality data via satellite. The primary reference gage is the top of the PVC well casing at 34.74 feet. The transducer is enclosed in a vertical two-inch PVC pipe on the west side of the building between gates 1 and 2 of the ASR intake building. Gage height was measured during April 2011 through December 2021. A YSI 6600 water-quality monitor equipped with water temperature, specific conductance, pH, dissolved oxygen, and turbidity (YSI Model 6136) sensors collected data during April 2011 through October 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 October 2015 through December 2021. A Hach Nitratax monitor collected nitrate data during March 2016 through December 2021.

Date model was developed: June 1, 2022

Model calibration data period: April 6, 2011 through October 29, 2021

Model Data

All data were collected using USGS protocols (U.S. Geological Survey, variously dated; Wagner and others, 2006; Sauer and Turnipseed, 2010) and are stored in the National Water Information System (NWIS) database (U.S. Geological Survey, 2022). Explanatory variables were evaluated individually and in combination. Potential explanatory variables included gage height, 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 59 concomitant values of discretely collected bromide and continuously measured specific conductance during April 2011 through October 2021. Discrete samples were collected over a range of gage height and specific conductance conditions. Three samples had concentrations that were below the minimum reporting level (<0.04 milligrams per liter) and a Tobit regression model was developed to compute estimates of bromide using the absolute maximum likelihood estimation approach (Hald, 1949; Cohen, 1950; Tobin, 1958; Helsel and others, 2020). Summary statistics and the complete model-calibration dataset are provided below. Outliers and influential points were identified using methods described in Rasmussen and others (2009), including leverage and Cook's distance (Cook's D; Cook, 1977) values. All samples were retained in the dataset.

Bromide

Discrete samples were collected near the northeast corner of the ASR intake building using 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 8 samples per year with a weighted basket sampler with a 1-Liter Teflon bottle or a DH-81 with a 1-Liter Teflon bottle, cap, and nozzle. Samples were analyzed for bromide by the Wichita Municipal Water and Wastewater Laboratory in Wichita, Kansas, or the USGS National Water Quality Laboratory according to standard methods (American Public Health Association and others, 1995).

Continuous Data

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

Model Development

Tobit regression models were developed using absolute maximum likelihood estimation methods using the *smwrQW* (v.0.7.9) package in R (version 4.0.0) programming language (R Core Team, 2020).

Specific conductance was selected as the best predictor of bromide based on residual plots, a larger pseudo coefficient of determination (pseudo R^2) and a relatively low estimated residual standard error (RSE). Specific conductance was positively related to bromide 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 bromide regression analysis at station 375350097262800:

Bromide-based model:

$$\log_{10}(BR) = 1.269 \times \log_{10}(SC) - 4.304$$

where,

\log_{10} = logarithm base 10;

BR = bromide, in milligrams per liter (mg/L); and

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

The log-transformed model may be retransformed to original units so that BR 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). Extracted model residuals used for BCF computation included censored residuals that were replaced by their expected values. For this model, the calculated BCF is 1.04.

Model Statistics, Data, and Plots

Model

$$\text{LOGBR} = + 1.269 * \text{LOGSC} - 4.304$$

Variable Summary Statistics

	BR	SC
Minimum	<0.04	88.0
1st Quartile	0.0591	247.8
Median	0.14	575.3
Mean	0.1663	556.7
3rd Quartile	0.2500	794.8
Maximum	0.58	1270.0

Explanatory Variables

Coefficients:

	Estimate	Std. Error	z-score	p-value
(Intercept)	-4.304	0.17574	-24.49	0
logSC	1.269	0.06504	19.52	0

Basic Model Statistics

Estimated residual standard error (Unbiased) = 0.137

Distribution: normal

Number of observations = 59, number censored = 3 (5.1 percent)

Loglik(model) = 32.36 Loglik(intercept only) = -32.23

Chi-square = 129.2, degrees of freedom = 1, p-value = <0.0001

Computation method: AMLE

Pseudo R-squared: 0.8901

AIC: -58.73

BIC: -52.5

Outlier Test Criteria

leverage cooksD

0.05085 0.70150

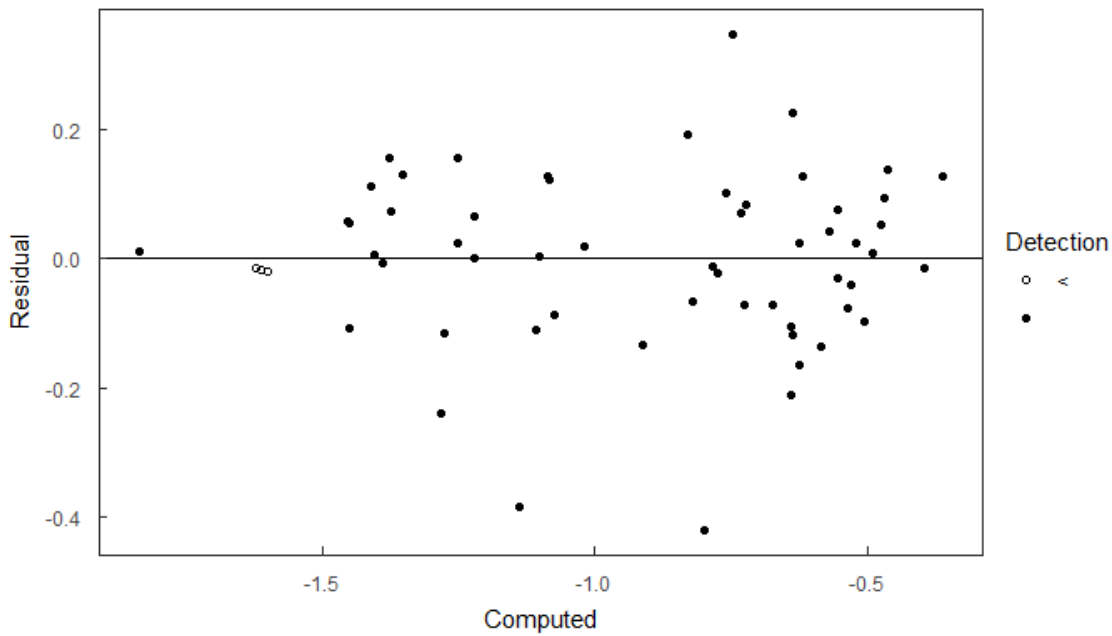
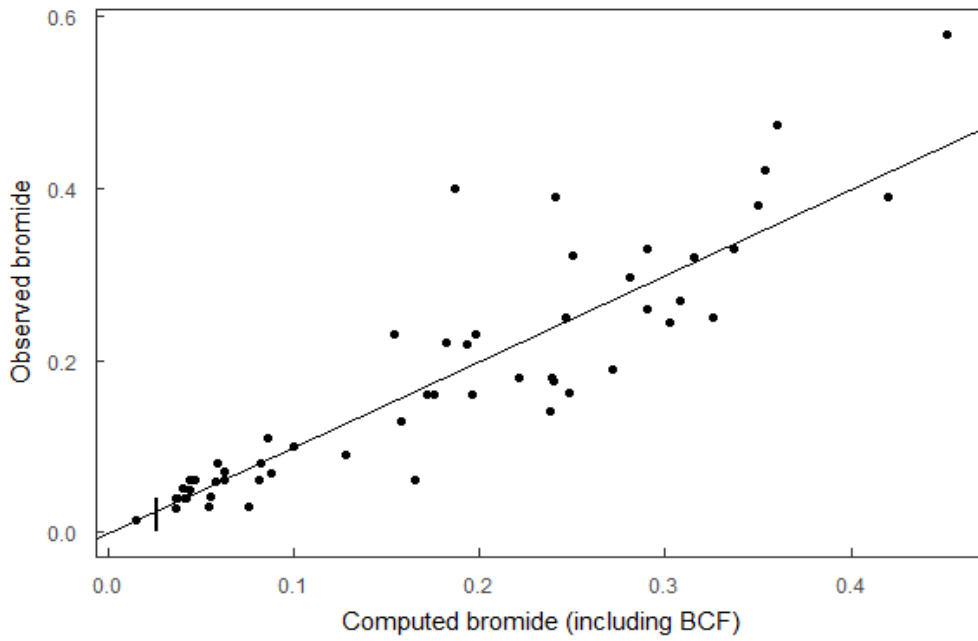
Flagged Observations

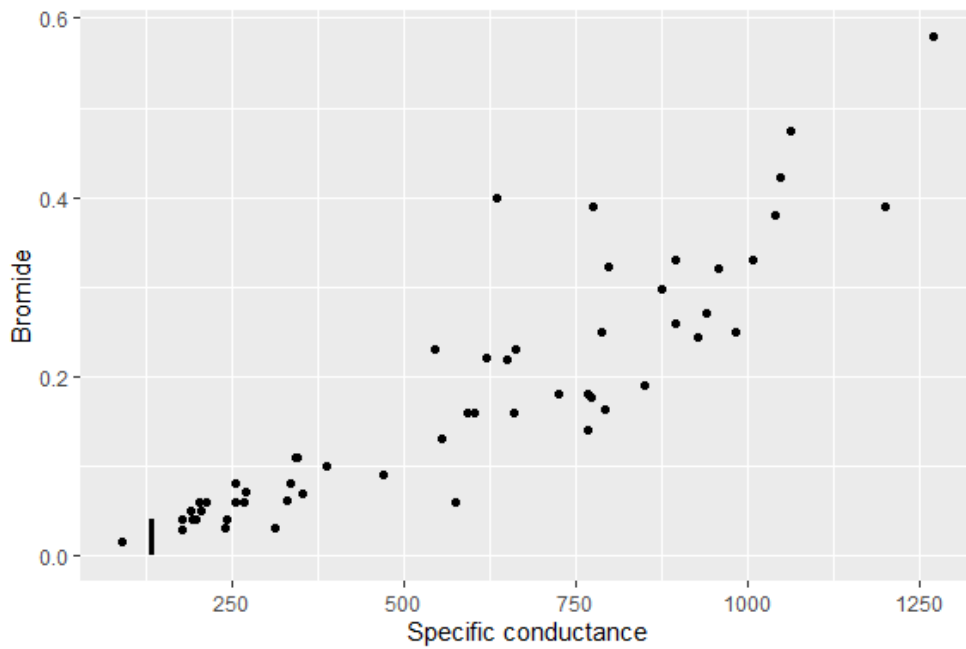
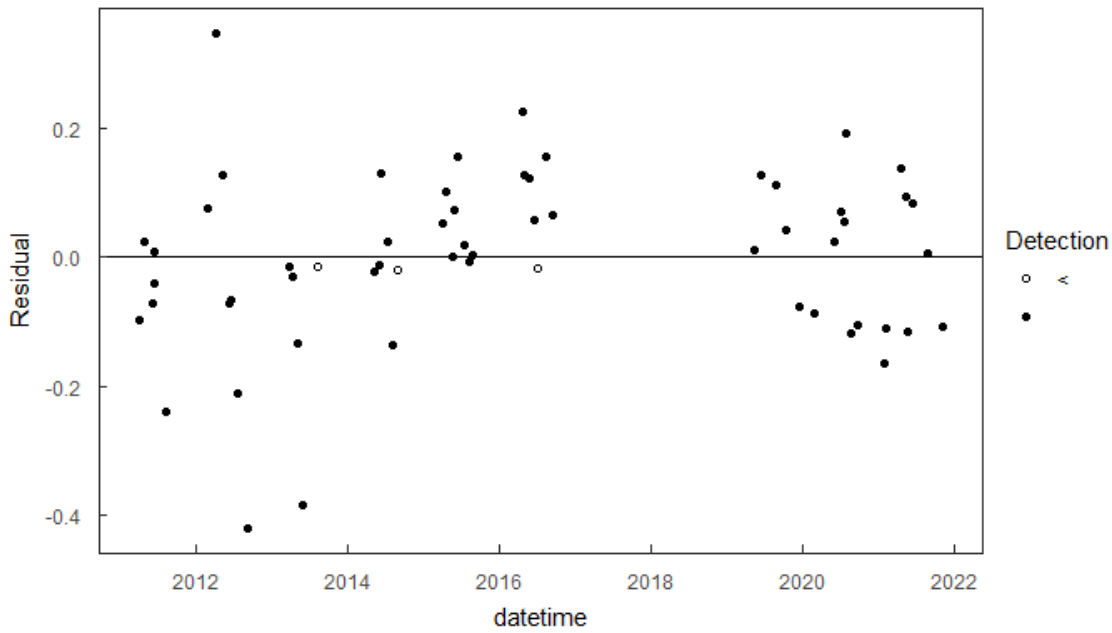
	logP71870	ycen	yhat	resids	leverage	cooksD
9	-0.2366	FALSE	-0.3641	0.12751	0.05462	0.0264584
18	-1.3979	TRUE	-1.6206	-0.01541	0.07114	0.0005213
24	-1.3979	TRUE	-1.5998	-0.01988	0.0679	0.0008222
37	-1.3979	TRUE	-1.6122	-0.01712	0.06982	0.0006296
40	-1.8239	FALSE	-1.8357	0.01177	0.11051	0.0005151

95% Confidence Intervals

	2.5 %	97.5 %
(Intercept)	-4.648372	-3.959474
logSC	1.141882	1.396835

Plots





Model-Calibration Dataset

	datetime	logP71870	logSC	P71870	SC	Computed logP71870	Computed P71870
1	4/6/2011 9:20:00	-0.602	2.99	0.25	983	-0.507	0.3252
2	5/2/2011 9:50:00	-0.495	2.98	0.32	957	-0.521	0.3145
3	6/7/2011 11:15:00	-0.745	2.86	0.18	725	-0.674	0.2211
4	6/20/2011 12:05:00	-0.481	3	0.33	1009	-0.492	0.3364
5	6/21/2011 9:30:00	-0.569	2.97	0.27	940	-0.531	0.3076
6	8/12/2011 8:50:00	-1.52	2.38	0.03	240	-1.284	0.0544
7	2/29/2012 11:45:00	-0.481	2.95	0.33	896	-0.558	0.2891
8	4/5/2012 9:45:00	-0.398	2.8	0.4	634	-0.748	0.1866
9	5/9/2012 9:00:00	-0.237	3.1	0.58	1270	-0.365	0.4503
10	6/12/2012 9:00:00	-0.796	2.82	0.16	659	-0.727	0.1959
11	6/19/2012 9:00:00	-0.886	2.74	0.13	555	-0.821	0.1575

12	7/19/2012	8:30:00	-0.854	2.89	0.14	768	-0.643	0.2377
13	9/11/2012	8:20:00	-1.22	2.76	0.06	575	-0.802	0.1649
14	3/27/2013	9:15:00	-0.409	3.08	0.39	1200	-0.397	0.4191
15	4/13/2013	16:35:00	-0.585	2.95	0.26	896	-0.557	0.2894
16	5/9/2013	11:00:00	-1.05	2.67	0.09	470	-0.913	0.1276
17	6/1/2013	9:55:00	-1.52	2.49	0.03	311	-1.14	0.0756
18	8/8/2013	9:00:00	<-1.4	2.11	<0.04	130	-1.621	0.025
19	5/14/2014	9:45:00	-0.796	2.78	0.16	604	-0.775	0.1752
20	6/3/2014	9:00:00	-0.796	2.77	0.16	593	-0.785	0.1713
21	6/9/2014	9:05:00	-1.22	2.32	0.06	211	-1.354	0.0463
22	7/15/2014	11:10:00	-0.602	2.9	0.25	789	-0.628	0.2461
23	8/4/2014	8:20:00	-0.721	2.93	0.19	850	-0.586	0.2707
24	9/3/2014	9:00:00	<-1.4	2.13	<0.04	135	-1.601	0.0262
25	4/6/2015	11:25:00	-0.42	3.02	0.38	1040	-0.475	0.3495
26	4/22/2015	11:00:00	-0.658	2.79	0.22	621	-0.76	0.1816
27	5/20/2015	9:15:00	-1.22	2.43	0.06	268	-1.223	0.0625
28	5/27/2015	9:10:00	-1.3	2.31	0.05	203	-1.376	0.044
29	6/17/2015	8:20:00	-1.22	2.3	0.06	202	-1.379	0.0436
30	7/13/2015	10:30:00	-1	2.59	0.1	387	-1.02	0.0997
31	8/6/2015	8:50:00	-1.4	2.3	0.04	197	-1.391	0.0424
32	8/27/2015	9:10:00	-1.1	2.52	0.08	333	-1.103	0.0824
33	4/21/2016	9:30:00	-0.409	2.89	0.39	775	-0.637	0.2406
34	5/3/2016	9:40:00	-0.959	2.53	0.11	342	-1.088	0.0853
35	5/26/2016	9:35:00	-0.959	2.54	0.11	345	-1.084	0.0862
36	6/17/2016	10:30:00	-1.4	2.24	0.04	176	-1.456	0.0365
37	7/6/2016	9:00:00	<-1.4	2.12	<0.04	132	-1.613	0.0255
38	8/11/2016	9:35:00	-1.1	2.4	0.08	253	-1.254	0.0582
39	9/13/2016	9:15:00	-1.15	2.43	0.07	268	-1.222	0.0626
40	5/9/2019	10:30:00	-1.82	1.94	0.015	88	-1.836	0.0152
41	6/12/2019	9:35:00	-0.491	2.9	0.322	798	-0.622	0.2495
42	8/20/2019	10:00:00	-1.3	2.28	0.0503	190	-1.412	0.0404
43	10/9/2019	10:20:00	-0.527	2.94	0.297	874	-0.571	0.2803
44	12/11/2019	9:50:00	-0.614	2.97	0.243	927	-0.539	0.3021
45	2/24/2020	12:40:00	-1.16	2.54	0.0692	351	-1.075	0.088
46	5/27/2020	9:50:00	-1.23	2.4	0.0591	253	-1.254	0.0582
47	6/30/2020	9:40:00	-0.661	2.81	0.218	650	-0.734	0.1925
48	7/17/2020	9:50:00	-1.4	2.25	0.0402	177	-1.451	0.0369
49	7/23/2020	9:00:00	-0.638	2.74	0.23	545	-0.832	0.1539
50	8/19/2020	9:50:00	-0.755	2.89	0.176	773	-0.639	0.2397
51	9/23/2020	9:20:00	-0.746	2.89	0.18	768	-0.642	0.238
52	1/27/2021	9:30:00	-0.789	2.9	0.163	792	-0.626	0.2473
53	2/3/2021	9:30:00	-1.22	2.52	0.0607	330	-1.108	0.0814
54	4/14/2021	9:50:00	-0.325	3.03	0.474	1063	-0.463	0.3594
55	5/12/2021	10:10:00	-0.375	3.02	0.422	1047	-0.472	0.3525
56	5/17/2021	10:10:00	-1.39	2.38	0.0406	242	-1.278	0.055
57	6/9/2021	11:20:00	-0.639	2.82	0.23	663	-0.723	0.1974
58	8/25/2021	11:30:00	-1.4	2.28	0.0399	192	-1.406	0.041
59	10/29/2021	10:30:00	-1.56	2.25	0.0276	176	-1.453	0.0368

Definitions

BR: Bromide in mg/L (71870)

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

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