Appendix 12. Model Archival Summary for Magnesium Concentration at Station 06892350; Kansas River at De Soto, Kansas

This model archival summary summarizes the magnesium concentration (Mg) model developed to compute 15-minute Mg from July 19, 2012 onward. This model supersedes all previous models.

Site and Model Information

Site number: 06892350
Site name: Kansas River at De Soto, Kansas
Location: Lat 38°59'00", long 94°57'52" referenced to North American Datum of 1927, in NE 1/4 SE 1/4 SE 1/4 sec.28, T.12 S., R.22 E., Leavenworth County, KS, Hydrologic Unit 10270104.

Equipment: An YSI 6600 water-quality monitor equipped with sensors for water temperature, specific conductance, dissolved oxygen, pH, turbidity, and chlorophyll was installed from August 2012 through May 2014. From June 2014 to the present (2015) a Xylem YSI EXO2 water-quality monitor equipped was installed with sensors for water temperature, specific conductance, dissolved oxygen, pH, turbidity, and chlorophyll. The monitor is housed in a 4-inch diameter galvanized steel pipe. Readings from the water-quality monitor are recorded every 15 minutes and transmits data by way of satellite, hourly.

Date model was created: October 15, 2015

Model calibration data period: July 19, 2012 – June 29, 2015

Model application date: July 19, 2012 onward

Model-Calibration Dataset

All data were collected using U.S. Geological Survey (USGS) protocols and are stored in the National Water Information System (NWIS) database. Linear regression models were developed using the open-source software package "R." Explanatory variables selected as inputs to linear regression were physicochemical properties: specific conductance, pH, water temperature, dissolved oxygen, turbidity, chlorophyll fluorescence, and streamflow. Seasonal components (sine and cosine variables) were also evaluated as explanatory variables in the models to determine if seasonal changes affected the model. All combinations of physicochemical properties and a seasonal component were evaluated to determine which combinations produced the best models.

The final selected regression model is based on 59 concurrent measurements of Mg concentration and specific conductance (SC) collected from July 19, 2012 through June 29, 2015. Samples were collected throughout the range of continuously observed hydrologic conditions. No samples were below laboratory detection limits. Summary statistics and the complete model-calibration dataset are provided below. Studentized residuals from the final model were inspected for values greater than 3 or less than negative 3. Values outside of that range are considered potential outliers and are investigated. One sample, June 11, 2014, was found to have potential errors in collection and processing, and has been removed from the dataset. All other potential outliers were not found to have errors associated with collection, processing, or analysis, and were therefore considered valid.

Magnesium Sampling Details

Cross-section samples are typically collected either from the downstream side of the bridge or instream within 100 feet of the bridge. The equal-width-increment (EWI) method is used, and samples typically are composited for analysis. Cross-section samples are collected every 2 weeks from March through October, once a month from November through February, and during selected runoff events. A FISP US DH-95, D-95, or D-96A1 depth integrating sampler is used from the bridge; and aDH-81 or DH-95 hand sampler is used for boat samples. Samples are analyzed for Mg concentration at the USGS National Water Quality Laboratory in Lakewood, Colorado.

Model Development

Regression analysis was done using R by examining SC, streamflow, and other continuously measured data as explanatory variables for estimating Mg concentration. A variety of models that predict Mg, $(Mg)^2$, $\sqrt{Mg}$ and models that predict $\log_{10}(Mg)$ were evaluated. The distribution of residuals was examined for normality, and plots of residuals (the difference between the measured and computed values) as compared to computed Mg were examined for homoscedasticity (meaning that their departures from zero did not change

substantially over the range of computed values). This comparison lead to the conclusion that the most appropriate and reliable model would be one that estimated $\log_{10}$(Mg).

SC was selected as the best predictor of Mg based on residual plots, relatively high adjusted coefficient of determination (adjusted R^2) and relatively low model standard percentage error (*MSPE*), prediction error sum of squares (PRESS), and Mallow's C_p. Values for all of the afore mentioned statistics and metrics were computed for various models and are included below along with all relevant sample data and more in-depth statistical information.

Model Summary

Summary of final regression analysis for Mg concentration at site number 06892350.

Mg concentration-based model:

$$\log_{10}(Mg) = 0.845 \times \log_{10}(SC) - 1.22$$

where

Mg = Magnesium in milligrams per liter (mg/L); and,

SC = specific conductance in microsiemens per centimeter at 25 degrees Celsius (µs/cm)

SC makes physical and statistical sense as explanatory variables for Mg.

The log-transformed model may be retransformed to the original units so that Mg 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). For this model, the calculated BCF is 1.00. The retransformed model, accounting for BCF is:

$$Mg = SC^{0.845} + 0.0602$$

Previous Models

Start year	End year	Model
2000	2005	$\log_{10}(Mg) = 0.954 \times \log_{10}(SC) - 1.54$

Magnesium Concentration Record

The Mg record is computed using this regression model and stored at the National Real-Time Water Quality (NRTWQ) Web site. Data are computed at 15-minute intervals. The complete water-quality record can be found at http://nrtwq.usgs.gov/ks.

Remarks

None

R Output for Magnesium; 06892350; Kansas River at De Soto, KS

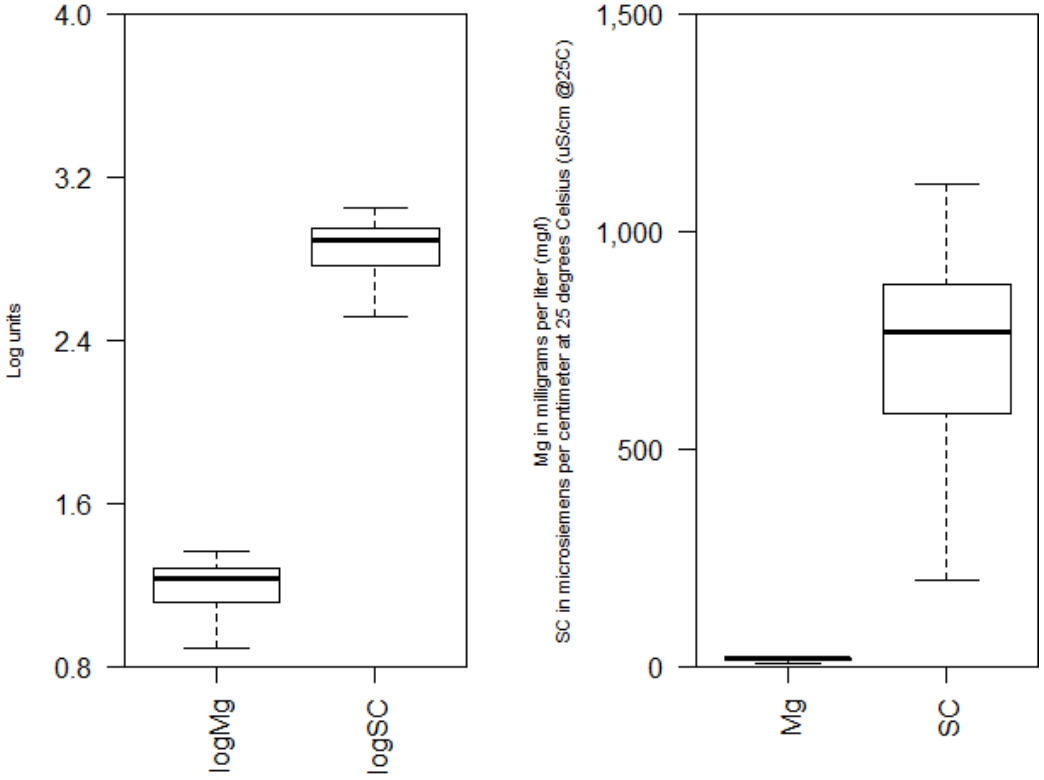
Model Form

logMg = + 0.845 * logSC + -1.22

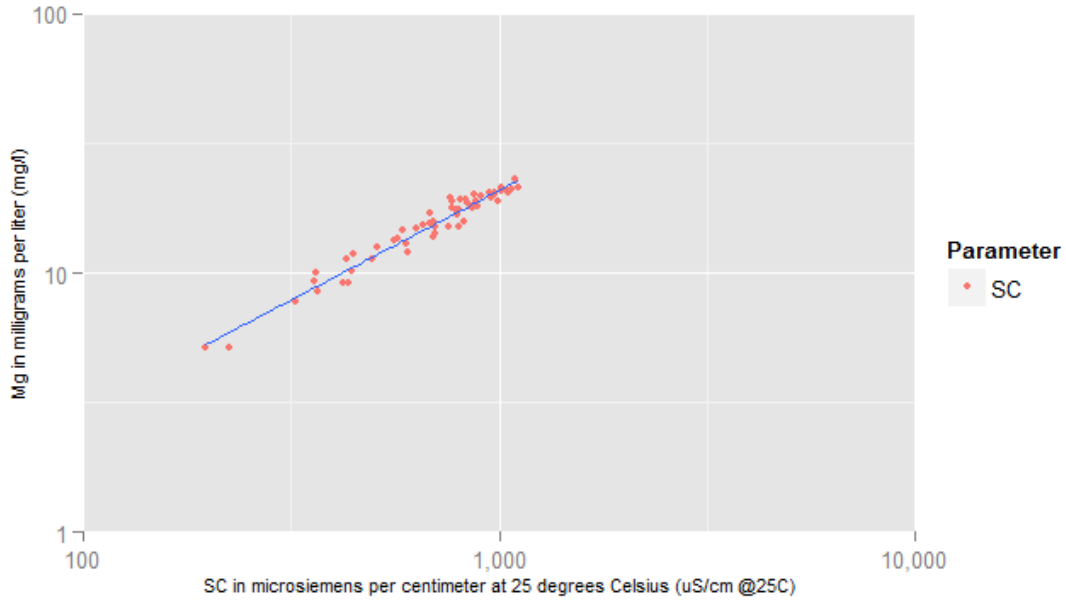
Variable Summary Statistics

	logMg	logSC	Mg	SC
Minimum	0.711	2.29	5.14	197
1st Quartile	1.110	2.76	12.90	569
Median	1.230	2.89	17.00	770
Mean	1.180	2.83	15.80	726
3rd Quartile	1.280	2.95	19.20	882
Maximum	1.360	3.05	23.10	1110

Box Plot(s) of sample data



Exploratory Plot



Model Calibration

Basic Data

```
Number of Observations                              59
Standard error (RMSE)                           0.0319
Upper Model standard percentage error (MSPE)      7.62
Lower Model standard percentage error (MSPE)      7.08
Coefficient of determination (R²)                0.952
Adjusted Coefficient of Determination (Adj. R²)  0.951
Bias Correction Factor (BCF)                        1
```

Explanatory Variables

```
            Coefficients Standard Error t value Pr(>|t|)
(Intercept)       -1.220         0.0711   -17.1 4.27e-24
logSC              0.845         0.0250    33.7 2.41e-39
```

Correlation Matrix

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

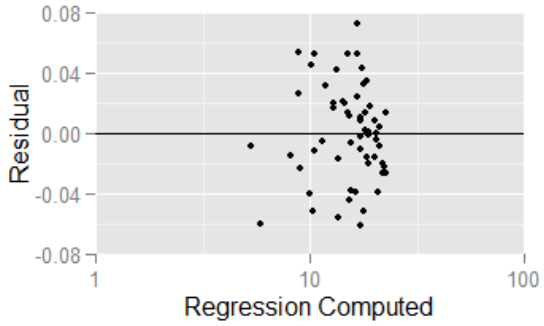
Test Criteria

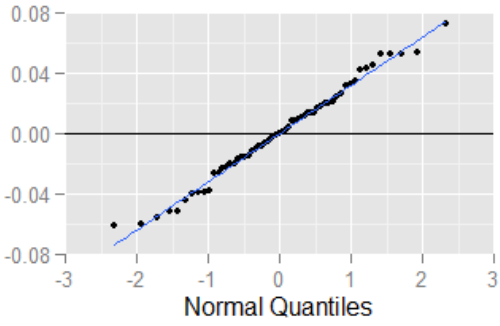
```
 Leverage   Cook's D     DFFITS
0.05084746 0.10555214 0.26037782
```

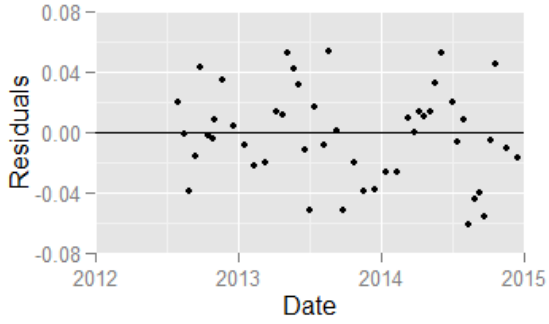
Flagged Observations

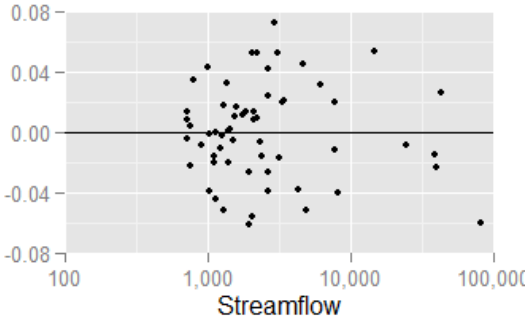
	logMg	Estimate	Residual	Standard Residual	Studentized Residual	Leverage	Cook's D	DFFITS
5/6/2013 12:30	1.0750	1.0220	0.052410	1.6750	1.7020	0.03794	0.05531	0.3381
7/1/2013 13:20	0.9606	1.0120	-0.051360	-1.6440	-1.6690	0.04085	0.05753	-0.3445
8/5/2013 11:30	0.7142	0.7227	-0.008507	-0.2974	-0.2950	0.19630	0.01080	-0.1458
8/19/2013 10:00	1.0010	0.9477	0.053180	1.7220	1.7530	0.06289	0.09949	0.4541
8/11/2014 15:10	1.1740	1.2360	-0.061540	-1.9480	-1.9990	0.01982	0.03836	-0.2842
9/8/2014 12:40	0.9605	1.0010	-0.040040	-1.2840	-1.2910	0.04424	0.03814	-0.2778
10/20/2014 14:00	1.0520	1.0070	0.045190	1.4470	1.4610	0.04226	0.04620	0.3070
1/12/2015 11:30	1.2910	1.2190	0.071800	2.2710	2.3610	0.01841	0.04837	0.3233
5/18/2015 15:30	0.8912	0.9064	-0.015230	-0.4979	-0.4946	0.08080	0.01090	-0.1466
6/6/2015 19:50	0.7105	0.7706	-0.060090	-2.0560	-2.1170	0.16050	0.40400	-0.9259
6/15/2015 14:50	0.9692	0.9428	0.026370	0.8546	0.8525	0.06486	0.02533	0.2245
6/29/2015 12:30	0.9271	0.9508	-0.023670	-0.7660	-0.7632	0.06167	0.01928	-0.1956

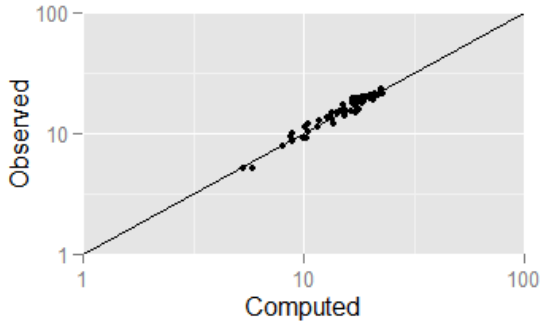
Statistical Plots

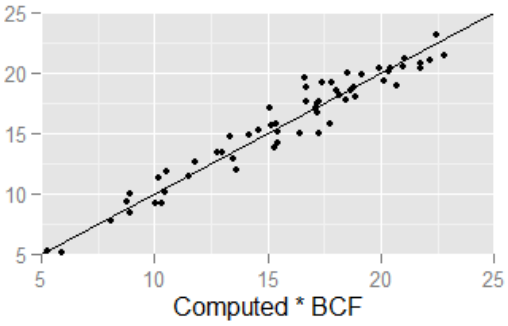


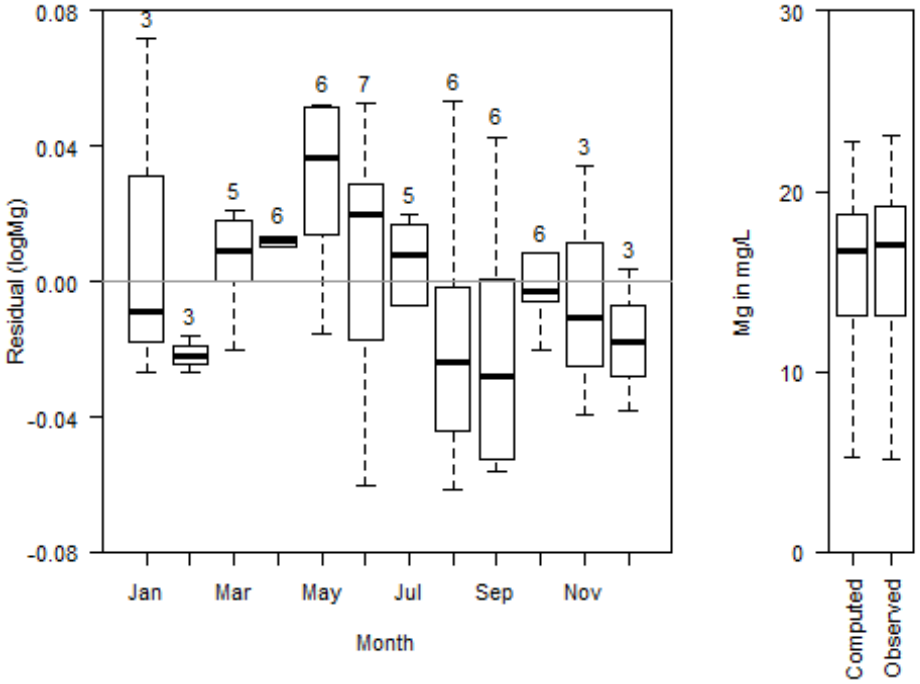


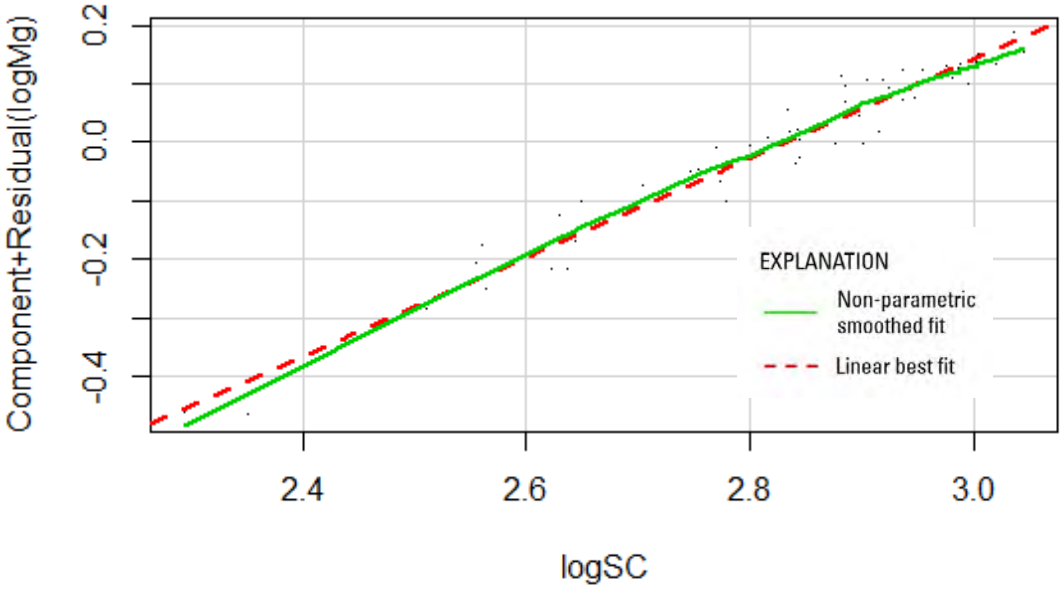









Residual (logMg)
0.08
0.04
0.00
-0.04
-0.08
3
3
5
6
6
7
5
6
6
6
3
3
Jan
Mar
May
Jul
Sep
Nov
Month
Mg in mg/L
30
20
10
0
Computed
Observed


Component+Residual(logMg)
0.2
0.0
-0.2
-0.4
2.4
2.6
2.8
3.0
logSC
EXPLANATION
Non-parametric smoothed fit
Linear best fit

Models considered

Model Formula	Number of Variables	Standard Error	R2	Adjusted R2	Cp	PRESS	VIF	MSPE
logMg ~ logSC	1	0.03191	95.23	95.14	4.743	0.0628	1	± 7.4
logMg ~ SC	1	0.05075	87.92	87.71	96.16	0.1663	1	± 12
logMg ~ logQ	1	0.07187	75.78	75.35	248.1	0.3219	1	± 17
logMg ~ SC + logSC	2	0.03098	95.58	95.42	2.332	0.06017	19.88	± 7.1
logMg ~ Q + logSC	2	0.031	95.57	95.41	2.408	0.06027	2.089	± 7.1
logMg ~ logQ + logSC	2	0.03192	95.3	95.14	5.761	0.06381	4.375	± 7.4
logMg ~ Q + SC + logSC	3	0.03089	95.68	95.45	3.043	0.05946	2.925	± 7.1
logMg ~ logQ + SC + logSC	3	0.03118	95.6	95.36	4.034	0.06153	4.594	± 7.2
logMg ~ Q + logQ + logSC	3	0.03123	95.59	95.35	4.235	0.06196	3.472	± 7.2
logMg ~ Q + logQ + SC + logSC	4	0.03117	95.68	95.36	5	0.0618	4.787	± 7.2

Data

	Date	logMg	logSC	Mg	SC	Computed logMg	Computed Mg	Residual	Normal Quantiles
1	2012-07-30	1.183	2.816	15.25	655	1.163	14.6	0.0199	0.633
2	2012-08-13	1.268	2.942	18.54	875.5	1.27	18.66	-0.00168	-0.0424
3	2012-08-27	1.175	2.877	14.97	753.2	1.215	16.43	-0.0394	-1.06
4	2012-09-10	1.249	2.938	17.76	866	1.266	18.49	-0.0163	-0.532
5	2012-09-24	1.282	2.906	19.14	805.3	1.239	17.39	0.0428	1.22
6	2012-10-15	1.231	2.898	17.01	791	1.233	17.13	-0.00186	-0.0848
7	2012-10-26	1.303	2.987	20.11	971	1.308	20.37	-0.00435	-0.127
8	2012-10-29	1.307	2.977	20.3	948	1.299	19.96	0.00853	0.213
9	2012-11-19	1.3	2.938	19.96	867	1.266	18.51	0.0339	1.06
10	2012-12-17	1.326	3.004	21.17	1010	1.322	21.05	0.00351	0.127
11	2013-01-14	1.313	3.003	20.54	1008	1.321	21.02	-0.00881	-0.301
12	2013-02-11	1.323	3.031	21.04	1075	1.345	22.19	-0.022	-0.74
13	2013-03-11	1.316	3.021	20.71	1050	1.336	21.76	-0.0203	-0.633
14	2013-04-08	1.363	3.037	23.09	1090	1.35	22.45	0.0133	0.391
15	2013-04-25	1.197	2.843	15.74	697	1.186	15.39	0.0108	0.345
16	2013-05-06	1.075	2.649	11.88	446	1.022	10.56	0.0524	1.55
17	2013-05-20	1.166	2.77	14.66	589.2	1.125	13.36	0.0416	1.13
18	2013-06-03	1.102	2.706	12.64	508	1.07	11.78	0.0316	0.919
19	2013-06-17	1.007	2.644	10.16	441	1.018	10.46	-0.0114	-0.391
20	2013-07-01	0.9606	2.637	9.133	433.5	1.012	10.31	-0.0514	-1.42
21	2013-07-15	1.129	2.755	13.45	569.4	1.112	12.98	0.0167	0.532
22	2013-08-05	0.7142	2.294	5.178	197	0.7227	5.295	-0.00851	-0.257
23	2013-08-19	1.001	2.561	10.02	363.8	0.9477	8.888	0.0532	1.93
24	2013-09-09	1.273	2.945	18.76	882	1.273	18.78	0.00073	0.0424
25	2013-09-23	1.196	2.917	15.71	826	1.248	17.77	-0.0523	-1.55
26	2013-10-21	1.254	2.947	17.94	886	1.274	18.85	-0.0203	-0.685
27	2013-11-18	1.276	2.996	18.86	990.6	1.315	20.71	-0.0396	-1.13
28	2013-12-16	1.15	2.846	14.12	701	1.188	15.47	-0.0384	-0.986
29	2014-01-13	1.33	3.045	21.37	1110	1.357	22.8	-0.027	-0.919
30	2014-02-10	1.31	3.021	20.4	1050	1.336	21.76	-0.0268	-0.856
31	2014-03-10	1.243	2.899	17.49	793.3	1.234	17.17	0.00919	0.257
32	2014-03-24	1.309	2.988	20.36	973.2	1.309	20.41	0.000166	0
33	2014-04-07	1.269	2.925	18.56	841.2	1.255	18.04	0.0134	0.437
34	2014-04-21	1.246	2.902	17.62	797.8	1.236	17.25	0.0103	0.301
35	2014-05-05	1.193	2.836	15.61	684.9	1.18	15.17	0.0137	0.484
36	2014-05-19	1.282	2.919	19.15	830.2	1.25	17.84	0.0318	0.986

37	2014-06-02	1.231	2.834	17.02	682.3	1.178	15.12	0.0526	1.71
38	2014-06-30	1.126	2.748	13.36	559.7	1.106	12.79	0.0201	0.685
39	2014-07-14	1.18	2.845	15.15	699.3	1.187	15.44	-0.00697	-0.213
40	2014-07-28	1.242	2.899	17.44	792.8	1.233	17.16	0.00817	0.17
41	2014-08-11	1.174	2.902	14.94	798.2	1.236	17.26	-0.0615	-2.32
42	2014-08-25	1.14	2.841	13.8	693.4	1.184	15.32	-0.0444	-1.31
43	2014-09-08	0.9605	2.623	9.131	420.2	1.001	10.04	-0.04	-1.22
44	2014-09-22	1.076	2.779	11.92	601.5	1.132	13.59	-0.0559	-1.71
45	2014-10-06	1.055	2.695	11.36	495.5	1.061	11.54	-0.00563	-0.17
46	2014-10-20	1.052	2.631	11.28	427.8	1.007	10.19	0.0452	1.31
47	2014-11-17	1.222	2.899	16.69	792.8	1.233	17.16	-0.011	-0.345
48	2014-12-15	1.111	2.775	12.9	595.1	1.128	13.47	-0.0176	-0.582
49	2015-01-12	1.291	2.883	19.55	763	1.219	16.61	0.0718	2.32
50	2015-02-09	1.287	2.981	19.35	958	1.303	20.14	-0.0161	-0.484
51	2015-03-09	1.299	2.955	19.89	902	1.281	19.14	0.0179	0.582
52	2015-03-23	1.172	2.801	14.85	633	1.151	14.19	0.0209	0.74
53	2015-04-06	1.26	2.928	18.19	848	1.258	18.16	0.00175	0.0848
54	2015-04-20	1.247	2.886	17.65	769.5	1.222	16.73	0.0243	0.797
55	2015-05-04	1.274	2.886	18.8	769.3	1.222	16.73	0.0518	1.42
56	2015-05-18	0.8912	2.512	7.784	325.1	0.9064	8.083	-0.0152	-0.437
57	2015-06-07	0.7105	2.351	5.135	224.5	0.7706	5.912	-0.0601	-1.93
58	2015-06-15	0.9692	2.555	9.315	359	0.9428	8.789	0.0264	0.856
59	2015-06-29	0.9271	2.565	8.455	366.9	0.9508	8.952	-0.0237	-0.797

Definitions and National Water Information System (parameter code)

Mg: Magnesium in mg/L (00925)
SC: Specific conductance in uS/cm @25C (00095)