Appendix 11. Model Archival Summary for Magnesium Concentration at Station 06887500; Kansas River at Wamego, 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: 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, KS, Hydrologic Unit 10270102.

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 regression model is based on 55 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. None of the Mg samples were deemed outliers.

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. Linear regression models were developed using the open-source software package “R.” Explanatory variables selected as inputs to linear regression were those physicochemical properties that were used in the logistic models: specific conductance, pH, water temperature, dissolved oxygen, turbidity, chlorophyll fluorescence, and streamflow. Seasonal components (sine and cosine variables) were used 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 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 a DH-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, $(Mg)^2$, √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 06887500.

Mg concentration-based model:

$$\log_{10}(Mg) = 0.768 \times \log_{10}(SC) - 0.996$$

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:

$$Mg = SC^{0.768} + 0.101$$

Previous Models

Start year	End year	Model
2000	2012	$\log_{10}(Mg) = 0.912 \times \log_{10}(SC) - 1.46$

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; 06887500; Kansas River at Wamego, KS

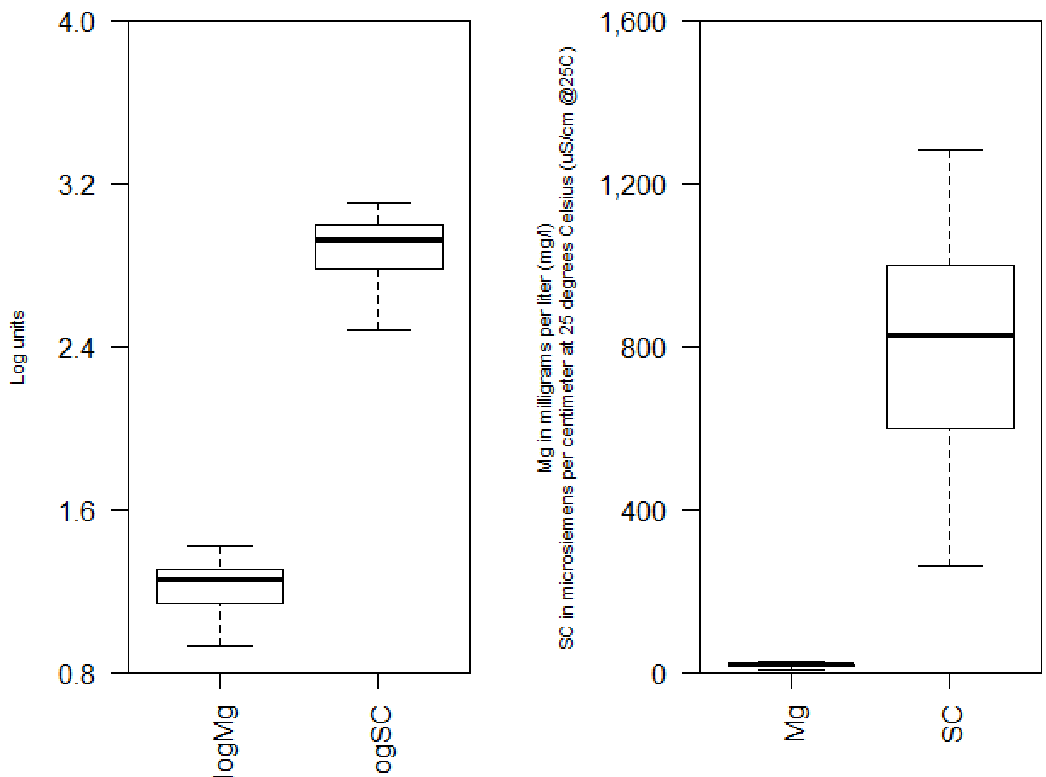
Model Form

logMg = + 0.768 * logSC + -0.996

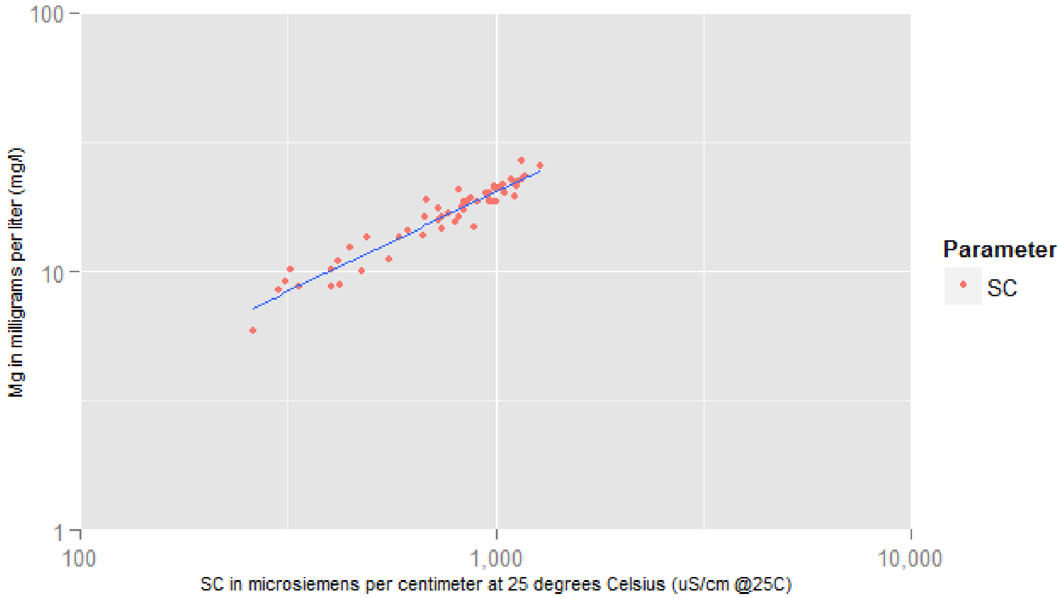
Variable Summary Statistics

	logMg	logSC	Mg	SC
Minimum	0.773	2.41	5.92	260
1st Quartile	1.130	2.77	13.50	585
Median	1.250	2.92	17.90	829
Mean	1.210	2.87	16.80	793
3rd Quartile	1.320	3.00	20.70	1000
Maximum	1.420	3.11	26.50	1280

Box Plot(s) of sample data



Exploratory Plot



Model Calibration

Basic Data

Number of Observations	55
Standard error (RMSE)	0.0408
Upper Model standard percentage error (MSPE)	9.86
Lower Model standard percentage error (MSPE)	8.98
Coefficient of determination (R^2)	0.92
Adjusted Coefficient of Determination (Adj. R^2)	0.919
Bias Correction Factor (BCF)	1

Explanatory Variables

	Coefficients	Standard Error	t value	Pr(>|t|)
(Intercept)	-0.996	0.0891	-11.2	1.46e-15
logSC	0.768	0.0310	24.8	8.41e-31

Correlation Matrix

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

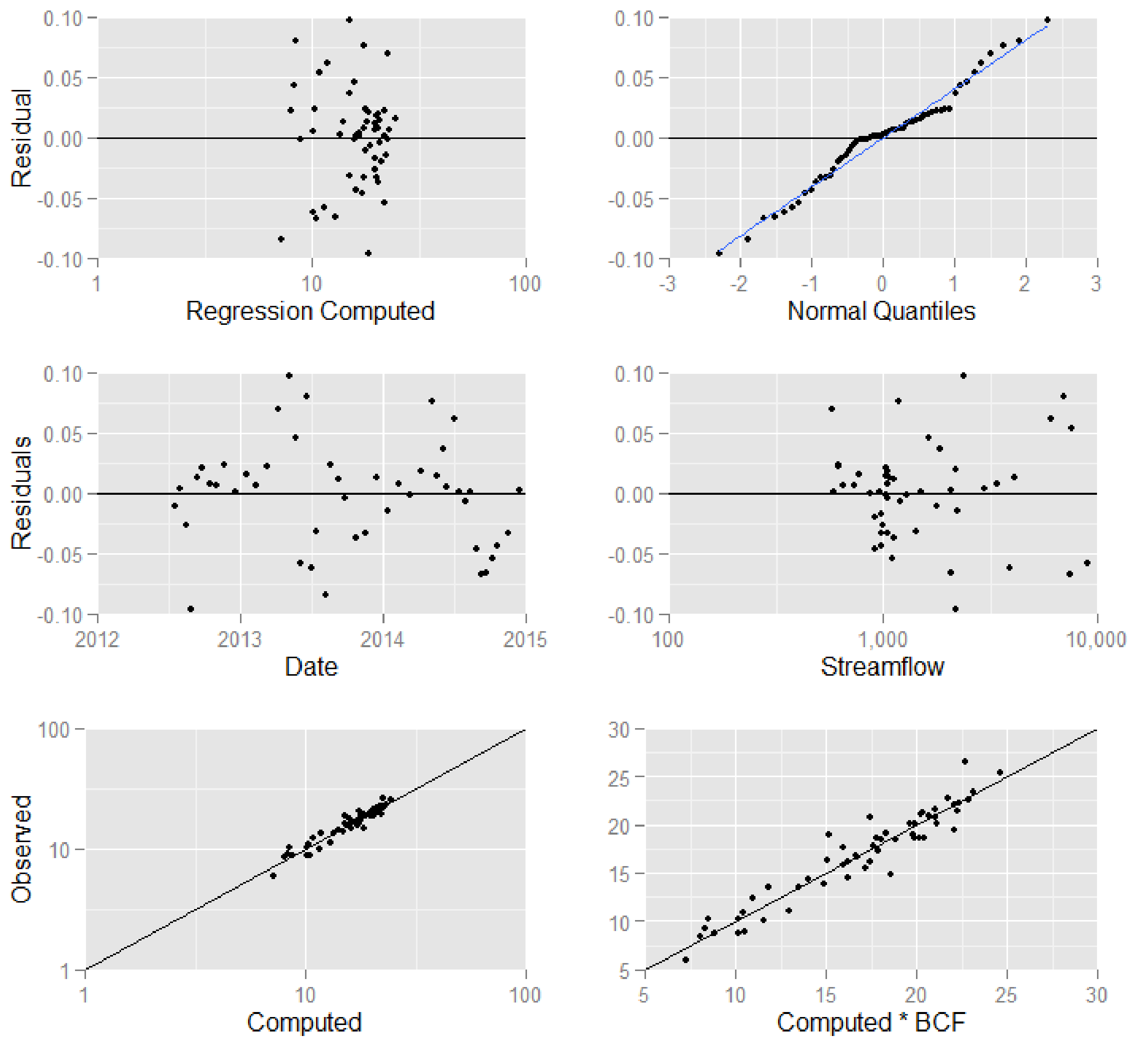
Test Criteria

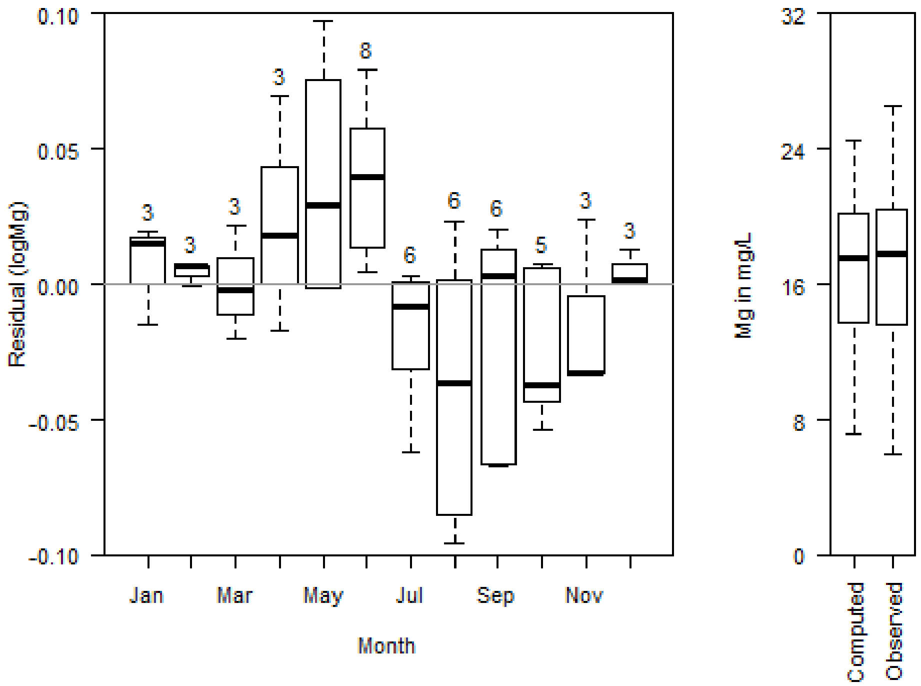
Leverage	Cook's D	DFFITS
0.05454545	0.10556635	0.26967994

Flagged Observations

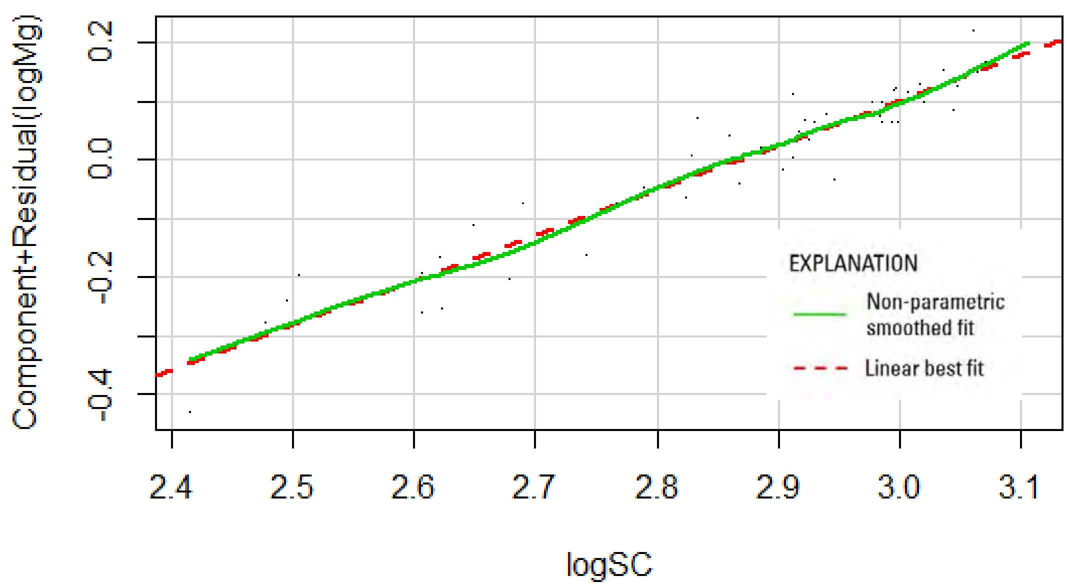
	logMg	Estimate	Residual	Standard Residual	Studentized Residual	Leverage	Cook's D	DFFITS
8/27/2012 11:20	1.1700	1.2660	-0.095860	-2.37300	-2.48600	0.02177	6.266e-02	-0.37090
4/8/2013 7:40	1.4240	1.3540	0.069440	1.73500	1.77000	0.03977	6.235e-02	0.36020
5/6/2013 8:00	1.2770	1.1800	0.097320	2.40600	2.52500	0.01884	5.556e-02	0.34990
6/3/2013 8:50	1.0030	1.0600	-0.057500	-1.43600	-1.45100	0.03887	4.171e-02	-0.29180
6/17/2013 8:30	1.0070	0.9276	0.079300	2.04000	2.10500	0.09374	2.151e-01	0.67680
7/1/2013 8:10	0.9431	1.0050	-0.061840	-1.56000	-1.58200	0.05752	7.423e-02	-0.39070
8/5/2013 7:30	0.7727	0.8578	-0.085060	-2.24100	-2.33400	0.13650	3.970e-01	-0.92770
5/5/2014 9:00	1.3160	1.2410	0.075860	1.87600	1.92300	0.01938	3.476e-02	0.27030
6/11/2014 9:00	1.0100	1.0050	0.004889	0.12330	0.12220	0.05752	4.641e-04	0.03018
6/30/2014 8:30	1.1320	1.0700	0.062080	1.54800	1.57000	0.03627	4.511e-02	0.30450
9/8/2014 8:00	0.9506	1.0180	-0.067490	-1.69800	-1.72900	0.05253	7.992e-02	-0.40720
9/22/2014 9:20	1.0430	1.1100	-0.066440	-1.64900	-1.67700	0.02713	3.793e-02	-0.28010
5/18/2015 10:30	0.9421	0.9435	-0.001417	-0.03627	-0.03593	0.08533	6.137e-05	-0.01097
6/1/2015 8:00	1.0910	1.0380	0.053720	1.34700	1.35700	0.04577	4.349e-02	0.29720
6/15/2015 7:50	0.9630	0.9202	0.042820	1.10400	1.10600	0.09781	6.606e-02	0.36430
6/29/2015 8:20	0.9274	0.9057	0.021640	0.56040	0.55680	0.10610	1.864e-02	0.19180

Statistical Plots





0.10
0.05
0.00
-0.05
-0.10
Residual (logMg)
3
3
3
3
8
6
6
6
5
3
3
Jan
Mar
May
Jul
Sep
Nov
Month
32
24
16
8
0
Mg in mg/L
Computed
Observed



Component+Residual(logMg)
0.2
0.0
-0.2
-0.4
2.4
2.5
2.6
2.7
2.8
2.9
3.0
3.1
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	0.04084	92.04	91.89	13.65	0.09739	1	± 9.4
logMg ~ SC	1	0.04909	88.5	88.29	42.42	0.1406	1	± 11
logMg ~ logQ	1	0.07439	73.6	73.1	163.5	0.3157	1	± 17
logMg ~ logSC + sin2DY	2	0.03629	93.84	93.6	1.086	0.07853	1.001	± 8.4
logMg ~ logSC + cos2DY	2	0.04109	92.1	91.79	15.21	0.09873	1.527	± 9.5
logMg ~ Q + logSC	2	0.0412	92.05	91.75	15.57	0.1019	2.882	± 9.5
logMg ~ SC + logSC + sin2DY	3	0.03615	94	93.65	1.755	0.08087	29.16	± 8.3
logMg ~ logQ + logSC + sin2DY	3	0.03635	93.93	93.58	2.282	0.08028	5.432	± 8.4
logMg ~ Q + logSC + sin2DY	3	0.03654	93.87	93.51	2.79	0.08315	3.022	± 8.4
logMg ~ logQ + SC + logSC + sin2DY	4	0.0364	94.04	93.56	3.454	0.08523	6.084	± 8.4
logMg ~ Q + SC + logSC + sin2DY	4	0.0365	94.01	93.53	3.708	0.09259	4.907	± 8.4
logMg ~ SC + logSC + sin2DY + cos2DY	4	0.03651	94	93.52	3.739	0.08205	31.9	± 8.4
logMg ~ Q + logQ + SC + logSC + sin2DY	5	0.0366	94.09	93.49	5.004	0.09401	7.528	± 8.4
logMg ~ logQ + SC + logSC + sin2DY + cos2DY	5	0.03677	94.04	93.43	5.441	0.08655	6.087	± 8.5
logMg ~ Q + SC + logSC + sin2DY + cos2DY	5	0.03686	94.01	93.4	5.695	0.09395	4.919	± 8.5
logMg ~ Q + logQ + SC + logSC + sin2DY + cos2DY	6	0.03698	94.09	93.35	7	0.09559	7.574	± 8.5

Data

0	Date	logMg	logSC	Mg	SC	Computed logMg	Computed Mg	Residual	Normal Quantiles
1	2012-07-19	1.24	2.925	17.36	842	1.25	17.85	-0.0103	-0.471
2	2012-07-30	1.223	2.886	16.73	770	1.22	16.67	0.00342	0.0454
3	2012-08-13	1.27	2.987	18.63	970	1.297	19.9	-0.0269	-0.686
4	2012-08-27	1.17	2.946	14.8	884	1.266	18.53	-0.0959	-2.29
5	2012-09-10	1.268	2.931	18.52	854	1.255	18.05	0.013	0.421
6	2012-09-24	1.282	2.941	19.15	872.3	1.262	18.35	0.0205	0.686
7	2012-10-15	1.252	2.918	17.87	828.7	1.245	17.64	0.00756	0.276
8	2012-10-29	1.303	2.987	20.1	970.5	1.297	19.91	0.00595	0.137
9	2012-11-19	1.272	2.923	18.69	837	1.248	17.77	0.0237	0.939
10	2012-12-17	1.343	3.045	22.01	1110	1.342	22.07	0.000582	-0.137
11	2013-01-14	1.405	3.107	25.4	1280	1.39	24.63	0.0153	0.522
12	2013-02-11	1.369	3.072	23.4	1180	1.362	23.14	0.00678	0.183
13	2013-03-11	1.358	3.037	22.79	1090	1.336	21.77	0.0218	0.806
14	2013-04-08	1.424	3.061	26.52	1151	1.354	22.7	0.0694	1.51
15	2013-05-06	1.277	2.834	18.92	682	1.18	15.19	0.0973	2.29
16	2013-05-20	1.246	2.861	17.62	726	1.2	15.93	0.0456	1.18
17	2013-06-03	1.003	2.678	10.06	476.6	1.06	11.53	-0.0575	-1.27
18	2013-06-17	1.007	2.506	10.16	320.3	0.9276	8.501	0.0793	1.9
19	2013-07-01	0.9431	2.606	8.773	404	1.005	10.16	-0.0618	-1.38
20	2013-07-15	1.141	2.824	13.83	667.5	1.172	14.94	-0.0316	-0.745
21	2013-08-05	0.7727	2.415	5.925	259.8	0.8578	7.238	-0.0851	-1.9
22	2013-08-19	1.04	2.621	10.96	418	1.016	10.43	0.0235	0.87
23	2013-09-09	1.302	2.979	20.04	952	1.291	19.62	0.0111	0.323
24	2013-09-23	1.316	3.017	20.7	1040	1.32	21	-0.00434	-0.372
25	2013-10-21	1.27	3	18.62	1000	1.307	20.37	-0.0373	-0.939
26	2013-11-18	1.27	2.994	18.62	987.2	1.303	20.17	-0.0329	-0.87
27	2013-12-16	1.159	2.79	14.41	616.3	1.146	14.05	0.0128	0.372
28	2014-01-13	1.33	3.049	21.38	1120	1.345	22.23	-0.015	-0.522
29	2014-02-10	1.32	3.007	20.9	1017	1.313	20.64	0.00729	0.229
30	2014-03-10	1.355	3.064	22.63	1160	1.357	22.83	-0.00205	-0.323
31	2014-04-07	1.322	2.996	21.01	991.4	1.304	20.24	0.0181	0.575

32	2014-05-05	1.316	2.913	20.72	818.7	1.241	17.47	0.0759	1.67
33	2014-05-19	1.334	3.017	21.57	1040	1.32	21	0.0135	0.471
34	2014-06-02	1.213	2.829	16.32	675.1	1.176	15.07	0.0365	1.01
35	2014-06-11	1.01	2.606	10.23	404	1.005	10.16	0.00489	0.0909
36	2014-06-30	1.132	2.69	13.54	490.3	1.07	11.79	0.0621	1.38
37	2014-07-14	1.21	2.872	16.2	744.4	1.209	16.24	0.000716	-0.0909
38	2014-07-28	1.268	2.957	18.52	905	1.274	18.87	-0.00631	-0.421
39	2014-08-11	1.223	2.888	16.71	773	1.221	16.72	0.00161	-0.0454
40	2014-08-25	1.188	2.905	15.43	803	1.234	17.22	-0.0457	-1.09
41	2014-09-08	0.9506	2.624	8.926	420.2	1.018	10.47	-0.0675	-1.67
42	2014-09-22	1.043	2.743	11.05	553.3	1.11	12.93	-0.0664	-1.51
43	2014-10-06	1.288	3.045	19.41	1110	1.342	22.07	-0.054	-1.18
44	2014-10-20	1.163	2.869	14.57	740	1.207	16.17	-0.0434	-1.01
45	2014-11-17	1.208	2.913	16.13	818.5	1.24	17.47	-0.0328	-0.806
46	2014-12-15	1.13	2.767	13.5	585.2	1.129	13.5	0.00175	0
47	2015-01-12	1.326	2.999	21.17	996.7	1.306	20.32	0.0196	0.63
48	2015-02-09	1.348	3.053	22.26	1130	1.348	22.38	-0.000468	-0.183
49	2015-03-09	1.303	3.02	20.07	1048	1.323	21.12	-0.0203	-0.63
50	2015-04-06	1.278	2.985	18.98	965.5	1.296	19.83	-0.0172	-0.575
51	2015-05-04	1.2	2.862	15.85	728	1.201	15.97	-0.00134	-0.229
52	2015-05-18	0.9421	2.526	8.752	336	0.9435	8.818	-0.00142	-0.276
53	2015-06-01	1.091	2.649	12.34	445.5	1.038	10.95	0.0537	1.27
54	2015-06-15	0.963	2.496	9.184	313.3	0.9202	8.357	0.0428	1.09
55	2015-06-29	0.9274	2.477	8.46	300	0.9057	8.083	0.0216	0.745

Definitions and National Water Information System (parameter code)

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