Appendix 11. Model Archive Summary for Magnesium Concentration at U.S. Geological Survey Station 07144790, Cheney Reservoir near Cheney, Kansas, during October 1, 2014, through September 30, 2021

This model archive summary summarizes the dissolved magnesium concentration model developed to compute 15-minute, hourly, or daily magnesium concentrations during October 1, 2014, onward. This model supersedes all prior models used during this period. The methods follow U.S. Geological Survey (USGS) guidance as referenced in relevant Office of Surface Water/Office of Water Quality Technical Memoranda and USGS Techniques and Methods, book 3, chapter C4 (Rasmussen and others, 2009; U.S. Geological Survey, 2016).

Any use of trade, firm, or product names is for descriptive purposes only and does not imply endorsement by the U.S. Government.

Site and Model Information

Site number: 07144790

Site name: Cheney Reservoir near Cheney, Kansas

Location: Lat 37°43'34", long 97°47'38" referenced to North American Datum of 1927, in SE 1/4 NE 1/4 NW 1/4 sec.06, T.27 S., R.4 W., Sedgwick County, Kans., hydrologic unit 11030014, in control house structure at outlet works of Cheney Dam on North Fork Ninnescah River, 6.0 mi north of Cheney, and at mile 15.9.

Equipment: A YSI, Inc., EXO water-quality monitor (YSI, Inc., 2017) equipped with sensors for water temperature, specific conductance, dissolved oxygen, pH, turbidity, chlorophyll fluorescence, and phycocyanin fluorescence was installed November 14, 2015. The EXO monitor is suspended from the dam intake tower walkway. The monitor is at a depth that fluctuates between three to six feet depending on reservoir elevation. Measurements from the EXO were recorded every 15 minutes to hourly and transmitted hourly via satellite. Reservoir elevation was measured using a Design Analysis H–350 nonsubmersible pressure transducer and H–355 gas system.

Date model was created: August 9, 2022

Model calibration data period: February 7, 2016, through August 31, 2021 (dataset consisted of 44 discrete water-quality samples).

Model application date: November 14, 2015, onward (date of EXO continuous water-quality monitor installation).

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Model Calibration Dataset

All data were collected using USGS protocols (U.S. Geological Survey, 2006; Wagner and others, 2006; Bennett and others, 2014) and are stored in the USGS National Water Information System database (https://doi.org/10.5066/F7P55KJN; U.S. Geological Survey, 2022). Potential explanatory variables evaluated individually and in combination were water temperature, specific conductance, pH, dissolved oxygen, turbidity, chlorophyll fluorescence, phycocyanin fluorescence, seasonality (sine and cosine variables), and reservoir elevation.

The regression model is based on 44 concomitant values of discretely collected magnesium concentration and continuously measured specific conductance during February 7, 2016, through August 31, 2021. Discrete samples were collected throughout the range of continuously observed hydrologic conditions. No samples had magnesium concentrations that were less than laboratory minimum reporting level. All potential explanatory variables were time interpolated within the 15-minute to hourly continuous record based on the discrete sample time. The maximum time span between two continuous data points used for interpolation was 4 hours (to preserve the sample dataset, field monitor averages obtained during sample collection were used for model development data if no continuous data were available or if gaps larger than 4 hours in the continuous data record resulted in missing interpolated data). Summary statistics and the complete model-calibration dataset are provided below. Potential outliers were identified using the methods described in Rasmussen and others (2009) and Helsel and others (2020). All potential outliers were investigated by reviewing sample collection information sheets and laboratory reports; if there were no clear issues, explanations, or conditions that would cause a result to be invalid for model calibration, the sample was retained in the dataset. Three samples in the model calibration dataset were flagged as outliers but all were retained in the dataset after further review.

Magnesium Sampling Details

Discrete water-quality samples were collected primarily by depth-integrating through the photic-zone (depth at which light is approximately 1 percent of that at the surface) using a double check-valve bailer (Lane and others, 2003). Vertical water-quality profiles collected during sampling indicated that thermal stratification rarely occurs, and water-quality conditions are typically uniform throughout the water column. Samples were collected from the walkway on the dam intake tower. Discrete samples were collected on a semifixed to event-based schedule six to eight times per year. All samples were collected between 9:15 a.m. and 12:20 p.m. Samples were analyzed for magnesium concentration by the Wichita Municipal Water and Wastewater Laboratory in Wichita, Kans., according to standard methods (Eaton and others, 1995).

Continuous Water-Quality Data

Specific conductance was continuously measured (15 minutes to hourly) using a YSI, Inc., EXO multiparameter sonde (YSI, Inc., 2017). The water-quality monitor was operated and maintained according to standard USGS methods (Wagner and others, 2006; Bennett and others, 2014). All continuous water-quality data at Cheney Reservoir near Cheney, Kans. are available in near-real time (updated hourly) from the USGS National Water Information System database

(https://doi.org/10.5066/F7P55KJN; U.S. Geological Survey, 2022) using the site number 07144790.

Model Development

Ordinary least squares linear regression was used to develop surrogate regression models that relate continuous water-quality conditions to discretely sampled constituent concentrations. All regressions were computed using the R software environment (R Core Team, 2020), The data and subsequent regression equation must meet the five assumptions necessary to apply ordinary least squares regression: the dependent variable is linearly related to the explanatory variables, data used to fit the model are representative of the data of interest, the variance of the residuals is constant (homoscedastic), the residuals are independent of the explanatory variables, and the residuals are normally distributed (Helsel and others, 2020). Previously published explanatory variables also were considered for continuity.

Specific conductance was selected as a good surrogate for magnesium concentration based on residual plots, coefficient of determination (R^2), and model standard percentage error (MSPE). Values for the aforementioned statistics were computed and are included below along with all relevant sample data and additional statistical information.

Model Summary

Summary of final magnesium concentration regression analysis at USGS site 07144790:

Magnesium concentration-based model:

$$Mg = 0.165 \times SPC + 0.728,$$

where,

Mg = magnesium, in milligrams per liter, dissolved; and

SPC = specific conductance, in microsiemens per centimeter at 25 degrees Celsius.

SPC makes physical and statistical sense as an explanatory variable for magnesium concentration because of its positive correlation with charged ionic species (Hem, 1985).

Extrapolation, defined as computation beyond the range of the model calibration dataset, may be used to extrapolate no more than 10 percent outside the range of the calibration data used to fit the model and is therefore limited. The extrapolation limit for magnesium concentration using this model is 18.7 milligrams per liter. The black vertical lines correspond to the censored results in the model calibration dataset as they are distributed in the model computations.

Model statistics, data, and plots

Definitions

Variable	Explanation
Cook's D	Cook's distance, a measure of influence (Helsel and others, 2020)
DFFITS	Difference in fits, a measure of influence (Helsel and others, 2020)

Variable	Explanation
E.vars	Explanatory variables
Leverage	An outlier's measure in the x direction (Helsel and others, 2020)
LOESS	Local polynomial regression fitting (Helsel and others, 2020)
Mg	Magnesium, milligrams per liter (mg/L), dissolved (USGS parameter code 00925)
MSE	Model standard error (Helsel and others, 2020)
MSPE	Model standard percentage error (Helsel and others, 2020)
Pr(>|*t*|)	The probability that the independent variable has no effect on the dependent variable (Helsel and others, 2020)
RMSE	Root mean square error (Helsel and others, 2020)
SPC	Specific conductance, in microsiemens per centimeter at 25 degrees Celsius (µS/cm at 25°C) (USGS parameter code 00095)
t value	Student's *t* value; the coefficient divided by its associated standard error (Helsel and others, 2020)

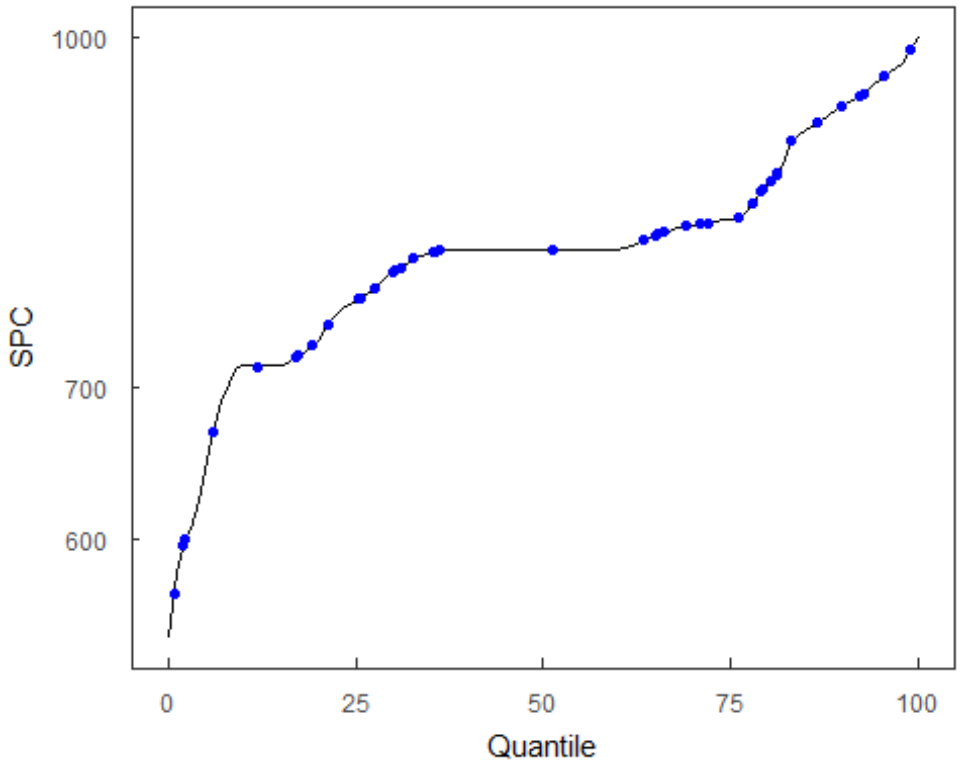
Model

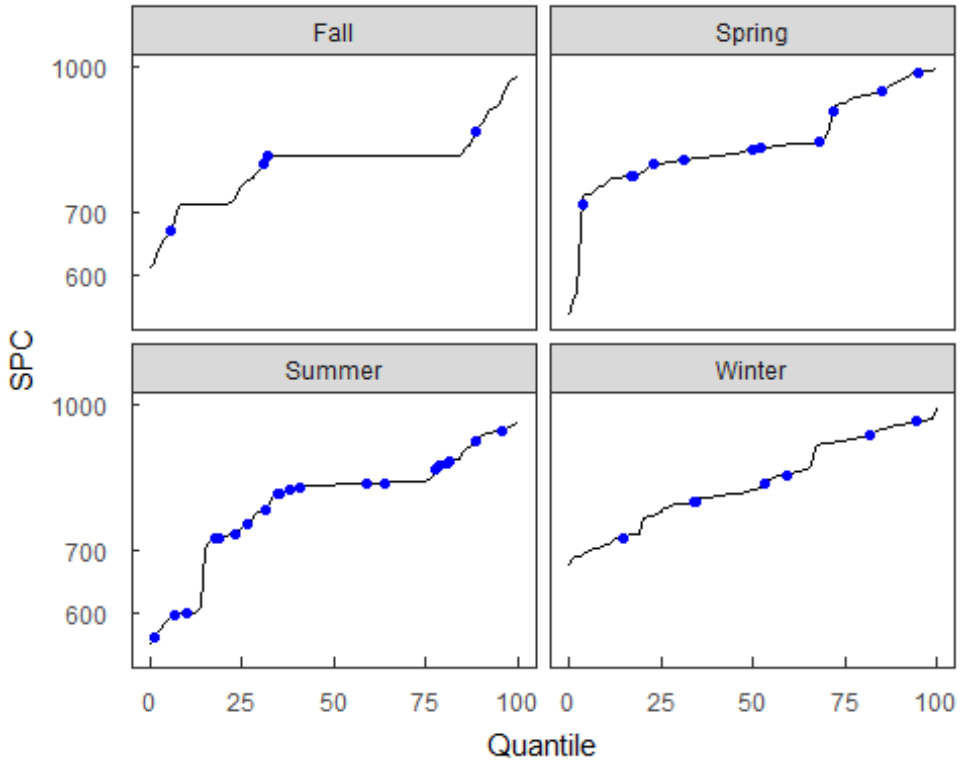
$$Mg = 0.165 \times SPC + 0.728$$

Variable summary statistics

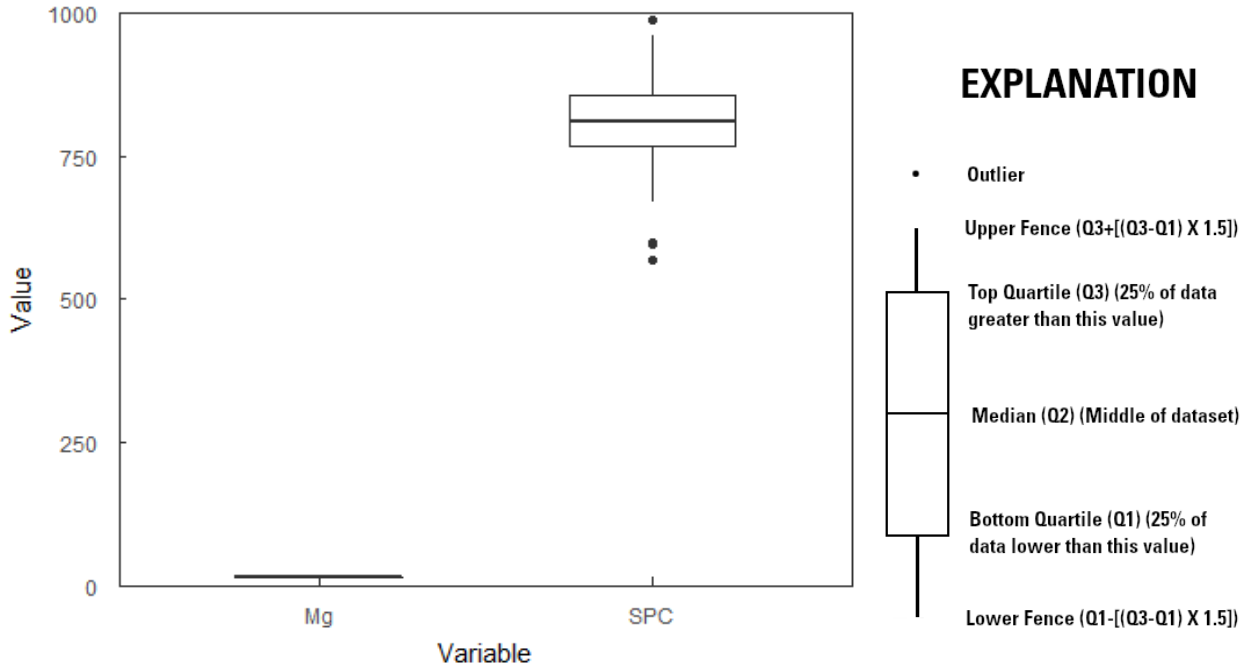
Variable	Minimum	Q1	Median	Mean	Q3	Maximum
Mg	10.5	13.1	14.1	14	15.4	17
SPC	568	767	810	805	855	988

Duration plots

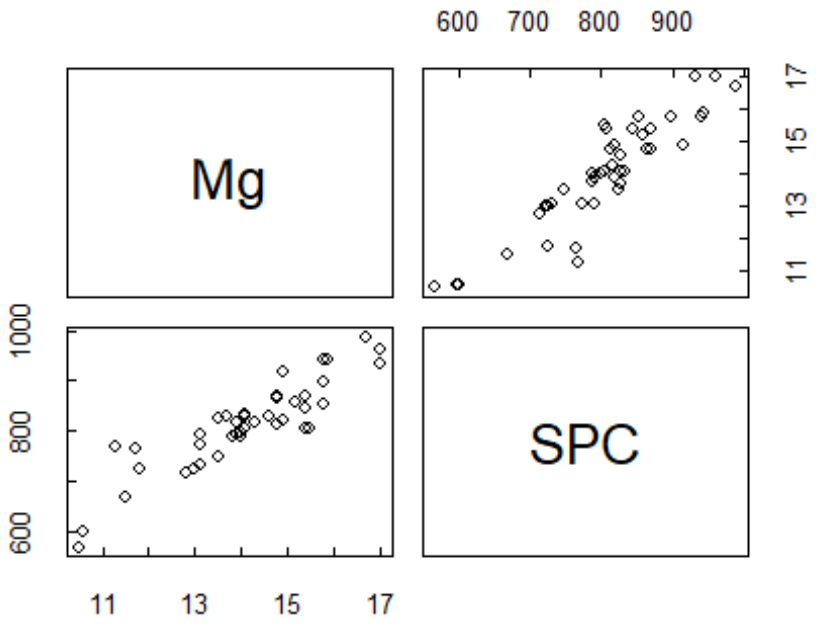




Box plots



Scatter plots



The x- and y-axis labels for a given bivariate plot are defined by the intersecting row and column labels.

Basic model statistics

Statistic	Value
Observations	44
R^2	0.814
Adjusted R^2	0.809
RMSE	0.729
Upper MSPE (90%)	5.19
Lower MSPE (90%)	-5.19

Model coefficients

	Estimate	Standard error	t value	Pr(>|t|)
(Intercept)	0.7277213	0.9898499	0.7351835	0.4663134
SPC	0.0165448	0.0012217	13.5427027	0.0000000

Correlation matrix

	Mg	SPC
Mg	1.0000000	0.9020358
SPC	0.9020358	1.0000000

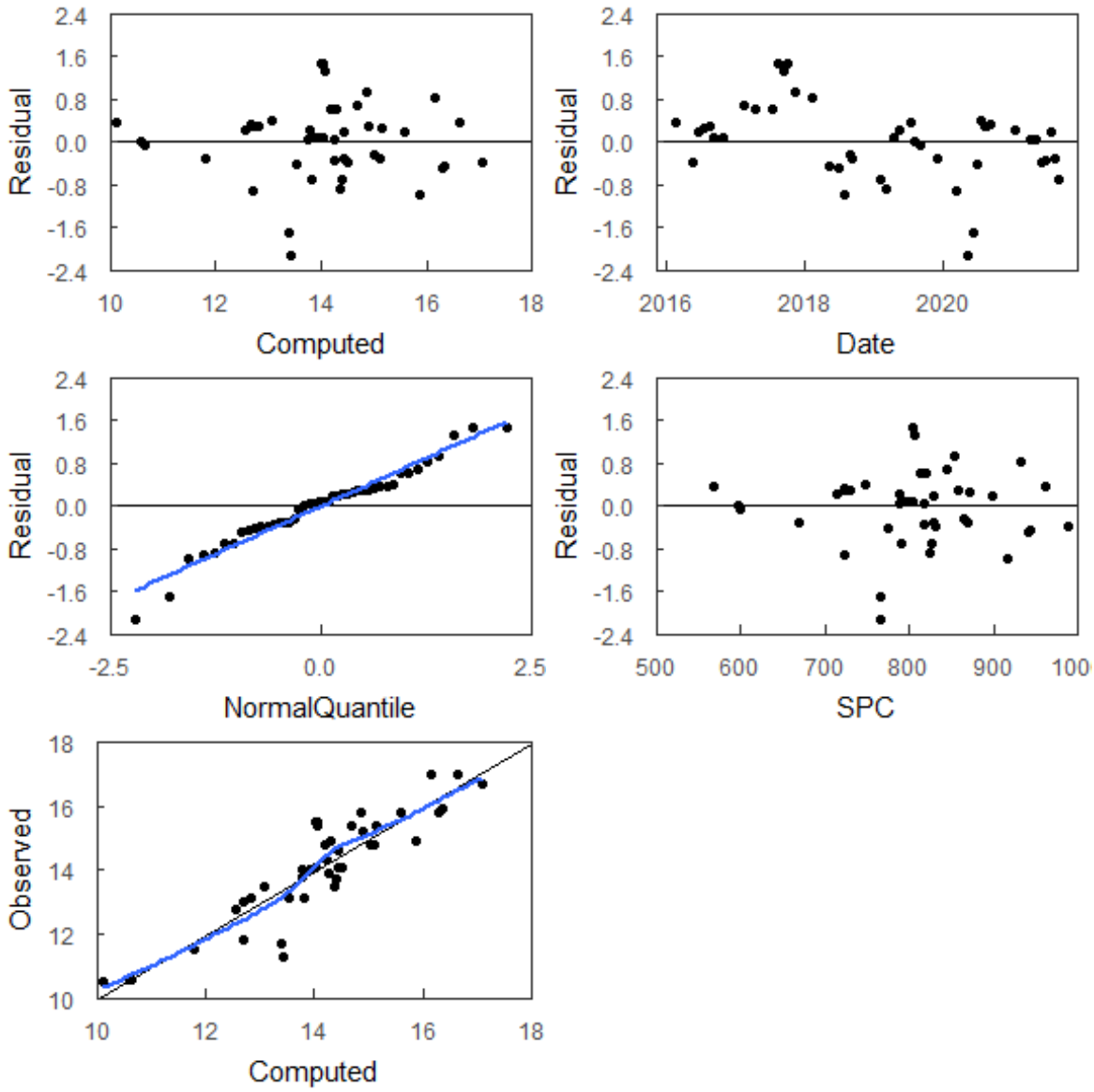
Outlier test criteria

Leverage	DFFITS	CooksD
0.1364	0.4264	0.1939

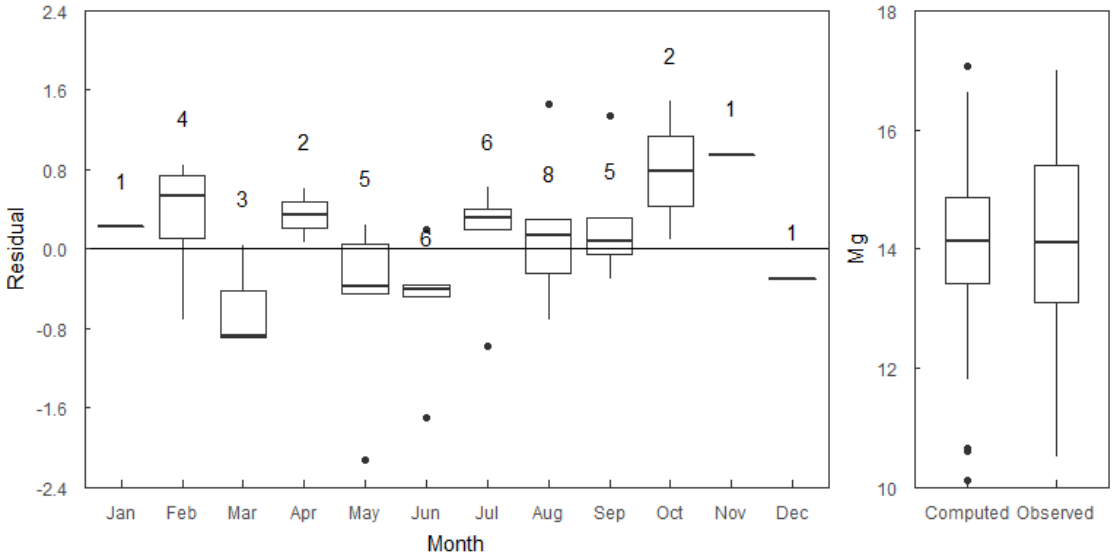
Flagged observations

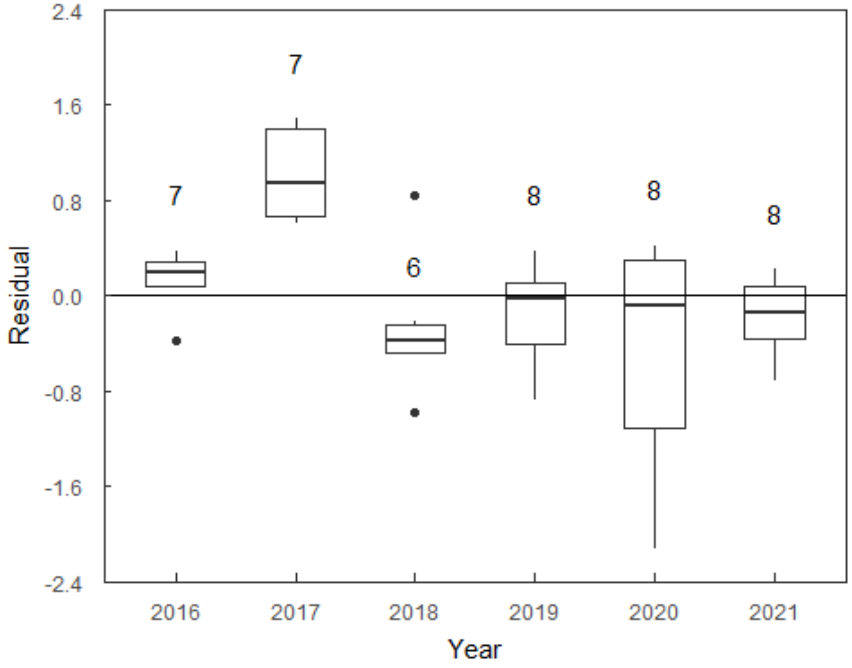
datetime	Mg	CooksD	DFFITS	Leverage	Studentized Residual
2019-07-09 10:15:00	10.5	0.0355	0.264	0.181	0.563
2019-08-06 11:00:00	10.6	4.54e-06	-0.00298	0.144	-0.00725
2019-09-03 10:40:00	10.6	0.000535	-0.0323	0.141	-0.0798

Statistical plots



The blue line shows the locally estimated scatterplot smoothing (LOESS). The black dots correspond to observed values. The black line represents the 1:1 line.





EXPLANATION

7 Number of values

Outlier

Upper Fence (Q3+[(Q3-Q1) X 1.5])

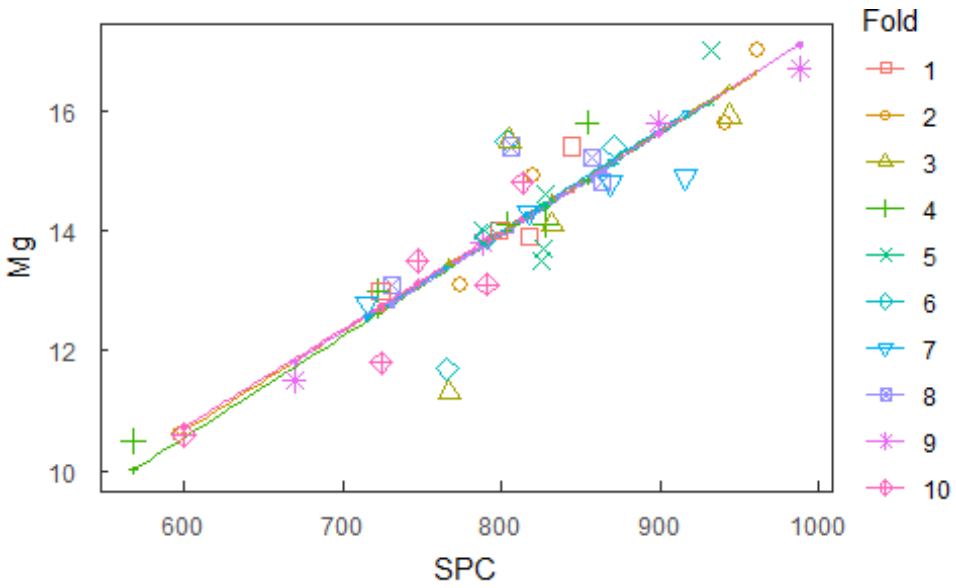
Top Quartile (Q3) (25% of data greater than this value)

Median (Q2) (Middle of dataset)

Bottom Quartile (Q1) (25% of data lower than this value)

Lower Fence (Q1-[(Q3-Q1) X 1.5])

Cross Validation



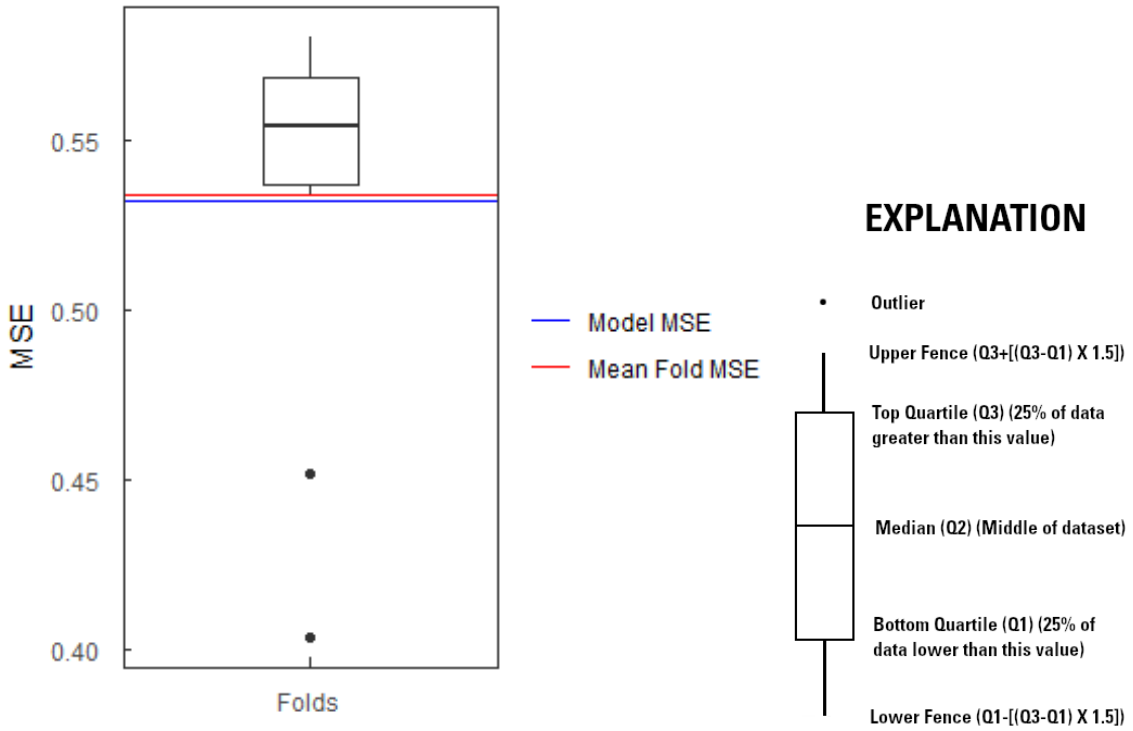
Fold - equal partition of the data (10 percent of the data).

Large symbols – observed value of a data point removed in a fold.

Small symbols – recomputed value of a data point removed in a fold.

Recomputed regression lines – adjusted regression line with one fold removed.

Statistic	Value
Minimum MSE of folds	0.404
25th Percentile	0.537
Median MSE of folds	0.554
Mean MSE of folds	0.534
75th percentile	0.569
Maximum MSE of folds	0.581
Model MSE	0.532



Model calibration dataset

datetime	Mg	SPC	Computed
2016-02-17 10:45:00	17.0	961	16.6
2016-05-17 10:20:00	16.7	988	17.1
2016-06-15 09:15:00	15.8	899	15.6
2016-07-18 10:40:00	15.4	871	15.1
2016-08-15 10:30:00	15.2	857	14.9
2016-09-06 10:40:00	14.1	804	14.0
2016-10-25 10:15:00	13.9	791	13.8
2017-02-09 10:40:00	15.4	844	14.7
2017-04-17 10:30:00	14.9	820	14.3
2017-07-10 11:40:00	14.8	813	14.2
2017-08-15 10:00:00	15.5	805	14.0
2017-09-07 10:00:00	15.4	806	14.1
2017-10-03 10:20:00	15.5	803	14.0
2017-11-13 12:00:00	15.8	854	14.9
2018-02-13 10:40:00	17.0	932	16.2
2018-05-08 10:30:00	15.9	944	16.3
2018-06-25 12:00:00	15.8	941	16.3
2018-07-26 11:40:00	14.9	916	15.9

datetime	Mg	SPC	Computed
2018-08-29 11:00:00	14.8	864	15.0
2018-09-11 09:40:00	14.8	869	15.1
2019-02-05 11:20:00	13.1	791	13.8
2019-03-07 10:50:00	13.5	825	14.4
2019-04-09 10:30:00	14	798	13.9
2019-05-14 11:10:00	12.8	715	12.6
2019-07-09 10:15:00	10.5	568	10.1
2019-08-06 11:00:00	10.6	597	10.6
2019-09-03 10:40:00	10.6	600	10.7
2019-12-04 10:50:00	11.5	669	11.8
2020-03-04 11:00:00	11.8	724	12.7
2020-05-06 10:30:00	11.3	767	13.4
2020-06-03 10:20:00	11.7	766	13.4
2020-06-25 11:30:00	13.1	774	13.5
2020-07-15 10:00:00	13.5	747	13.1
2020-08-04 11:30:00	13.1	731	12.8
2020-08-18 11:40:00	13.0	724	12.7
2020-09-01 10:50:00	13.0	723	12.7
2021-01-13 10:30:00	14.0	789	13.8
2021-03-31 10:30:00	13.8	788	13.8
2021-05-04 10:20:00	14.3	817	14.2
2021-06-03 10:30:00	14.1	832	14.5
2021-06-21 11:00:00	13.9	818	14.3
2021-07-20 10:40:00	14.6	828	14.4
2021-08-10 10:00:00	14.1	828	14.4
2021-08-31 11:40:00	13.7	827	14.4

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