Appendix 27. Model Archival Summary for *Escherichia coli* Bacteria Density at U.S. Geological Survey Site 06887500, Kansas River at Wamego, Kansas, during September 2013 through September 2019

This model archival summary summarizes the *Escherichia coli* bacteria (ECB; U.S. Geological Survey [USGS] parameter code 90902) density model developed to compute 15-minute ECB densities from September 2013 onward. This model supersedes all previous models.

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: 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, Kans., hydrologic unit 10270102.

Equipment: A YSI 6600 water-quality monitor equipped with sensors for water temperature, specific conductance, dissolved oxygen, pH, and turbidity (TBY) was installed from August 2012 through June 2014. A Xylem YSI EXO2 water-quality monitor equipped with sensors for water temperature, specific conductance, dissolved oxygen, pH, TBY, and chlorophyll and phycocyanin fluorescence was installed during June 2014 through September 2019. The monitor was housed in a 4-inch-diameter galvanized steel pipe. Readings from the water-quality monitor were recorded every 15 minutes and transmitted by way of satellite, hourly.

Date model was created: May 5, 2020

Model calibration data period: September 23, 2013, through September 23, 2019

Model application date: September 23, 2013, onward

Model-Calibration Dataset

All data were collected using USGS protocols (Wagner and others, 2006; U.S. Geological Survey, variously dated) and are stored in the National Water Information System (U.S. Geological Survey, 2020) database and available to the public. Ordinary least squares analysis was used to develop regression models using R programming language (R Core Team, 2020). Potential explanatory variables that were evaluated individually and in combination included streamflow, water temperature, specific conductance, dissolved oxygen, pH, TBY, and chlorophyll and phycocyanin fluorescence. These potential explanatory variables were interpolated within the 15-minute continuous record based on sample time. The maximum time span between two continuous data points used for interpolation was 2 hours (in order 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 1 hour in the continuous data record resulted in missing interpolated data). Seasonal components (sine and cosine variables) were also evaluated as potential explanatory variables.

The final selected regression model was based on 78 concurrent measurements of ECB density and sensor-measured TBY during September 23, 2013, through September 23, 2019. Samples were collected throughout the range of continuously observed hydrologic conditions. No samples had densities below laboratory detection limits. Forty-two sample densities were qualified as "estimated." Summary statistics and the complete model-calibration dataset are provided below. Potential outliers were identified using the methods described in Rasmussen and others (2009). Additionally, studentized residuals from the final model were inspected for values greater than three or less than negative three. Values outside of that range were considered potential outliers and were investigated. All potential outliers were not found to have errors associated with collection, processing, or analysis and were therefore considered valid.

This model is specific to the Kansas River at Wamego, Kans., during this study period and cannot be applied to data collected from other sites on the Kansas River or data collected from other waterbodies.

Escherichia coli Bacteria Sampling Details

Indicator bacteria samples typically were collected either from the downstream side of the bridge or instream within 100 feet of the bridge. The grab sample collection method with weighted basket was used for all indicator bacteria samples (contrary to the equal-width-increment collection method used for all other analytes; U.S. Geological Survey, variously dated). During July 2012 through June 2017, grab samples were collected every 2 weeks during March through October, once a month during November through February, and during selected reservoir release and runoff events. During July 2017 through September 2019, grab samples were

collected on a monthly to bimonthly basis, depending on flow conditions. An open-mouth bottle with weighted-basket sampler was used. Additional detail on sample collection is available in Foster and Graham (2016) and Graham and others (2018). Samples were analyzed for ECB density at the USGS Kansas Water Science Center in Lawrence, Kans.

Model Development

Ordinary least squares regression analysis was done using R programming language (R Core Team, 2020) to relate discretely collected ECB density to sensor-measured TBY. The distribution of residuals was examined for normality, and the plots of residuals (the difference between the measured and computed values) were examined for homoscedasticity (departures from zero did not change substantially over the range of computed values). Previously published explanatory variables were also strongly considered for continuity.

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

Model Summary

The following is a summary of final regression analysis for ECB density at USGS site 06887500:

ECB density -based model:

$$\log ECB = 1.27 \times \log TBY - 0.304$$

where

log = logarithm base 10;

ECB = Escherichia coli bacteria density, in colonies per 100 milliliters; and

TBY = turbidity, in formazin nephelometric units.

TBY makes physical and statistical sense as an explanatory variable for ECB because of its positive correlation with suspended material to which fecal indicator bacteria can physically bind.

The logarithmically (log) transformed model may be retransformed to the original units so that ECB 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 1.90. The retransformed model, accounting for BCF is as follows:

$$ECB = 1.90 \times (TBY^{1.27} \times 10^{-0.304})$$

Previous Models

Start Year	End Year	Model Equation	Reference
1999	2003	logECB = 1.15logTBY - 0.425	Rasmussen and others (2005)

Model Statistics, Data, and Plots

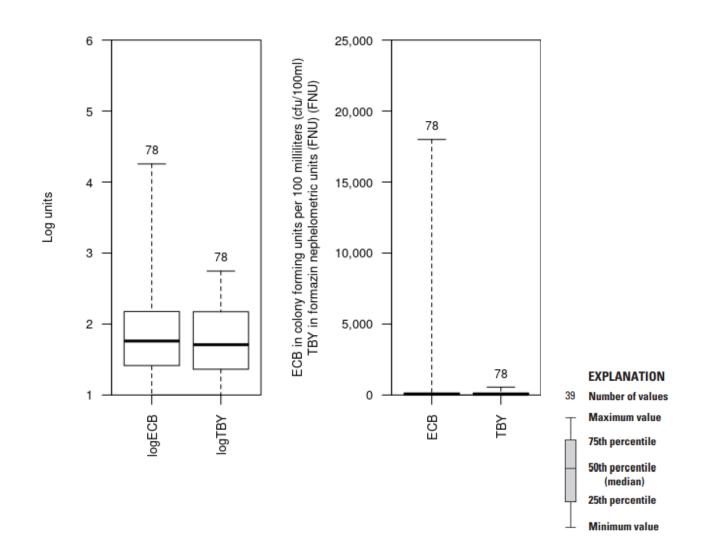
Model

logECB = + 1.27 * logTBY - 0.304

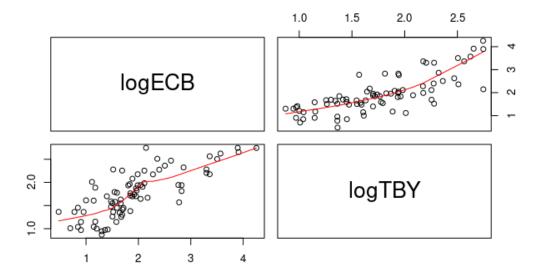
Variable Summary Statistics

	logECB	ECB	logTBY	TBY
Minimum	0.477	3	0.87	7.42
1st Quartile	1.410	26	1.36	23.10
Median	1.760	58	1.71	51.10
Mean	1.920	734	1.75	107.00
3rd Quartile	2.180	150	2.17	149.00
Maximum	4.260	18000	2.75	557.00

Box Plots



Exploratory Plots



Red line shows the locally weighted scatterplot smoothing (LOWESS).

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

Basic Model Statistics

Number of Observations	78
Standard error (RMSE)	0.513
Average Model standard percentage error (MSPE)	148
Coefficient of determination (R ²)	0.603
Adjusted Coefficient of Determination (Adj. R ²)	0.598
Bias Correction Factor (BCF)	1.9

Explanatory Variables

	Coefficients	Standard Er	ror t	value	Pr(> t)
(Intercept)	-0.304	0.	215	-1.42	1.61e-01
logTBY	1.270	0.	118	10.70	6.76e-17

Correlation Matrix

,	Intercept	E.vars
Intercept	1.000	-0.963
E.vars	-0.963	1.000

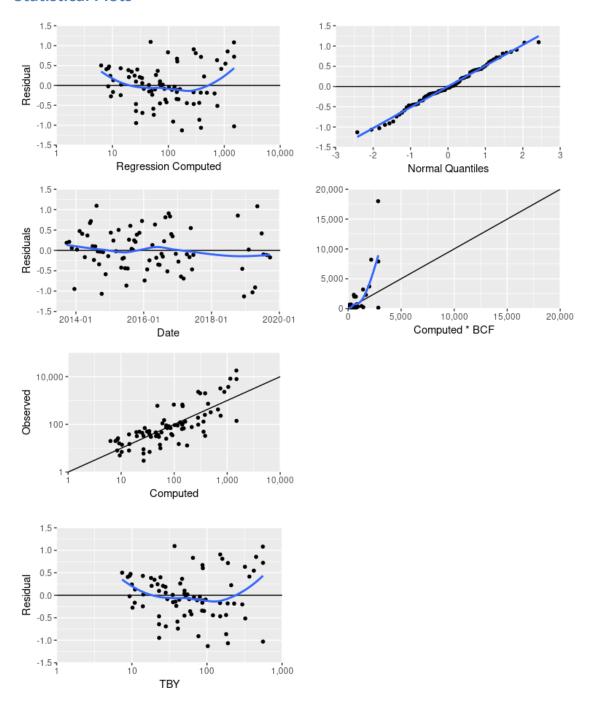
Outlier Test Criteria

Leverage Cook's	DFFITS
0.0769 0.194	

Flagged Observations

	logECB	Estimate	Residual	Standard Residual	Studentized Residual	. Leverage	Cook's D DFFI1
201410060900	1.52	2.58	-1.070	-2.10	-2.1	0.0274	0.0624 -0.36
201512140916	3.90	3.18	0.722	1.45	1.46	0.0649	0.0733 0.38
201810110940	3.91	3.06	0.855	1.71	1.74	0.0557	0.0865 0.42
201903180940	2.15	3.18	-1.030	-2.07	-2.12	0.0649	0.1490 -0.55
201905091520	4.26	3.17	1.080	2.18	2.24	0.0647	0.1640 0.58

Statistical Plots



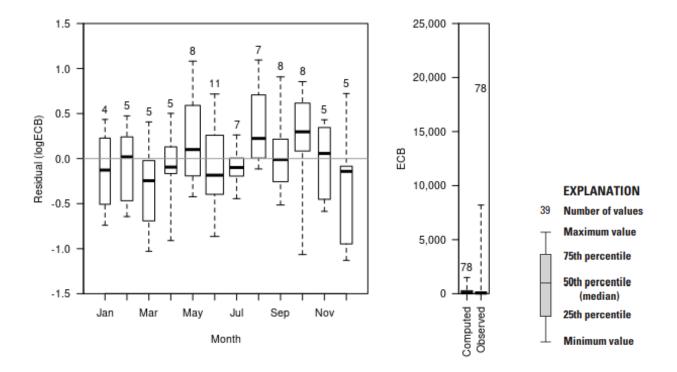
First row (left): Residual ECB related to regression computed ECB with local polynomial regression fitting, or locally estimated scatterplot smoothing (LOESS), indicated by the blue line.

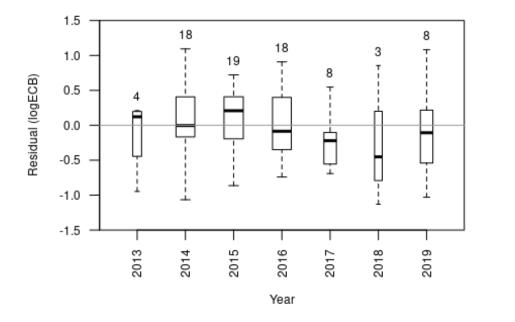
First row (right): Residual ECB related to the corresponding normal quantile of the residual with simple linear regression, indicated by the blue line.

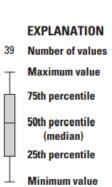
Second row: Residual ECB related to date (left) and regression computed ECB multiplied by the BCF (right) with LOESS, indicated by the blue line.

Third row: Observed ECB related to regression computed ECB.

Fourth row: Residual ECB related to TBY with LOESS, indicated by the blue line.

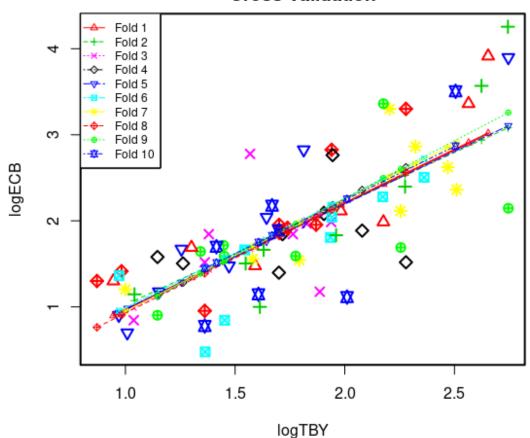






Cross-Validation

Cross-validation



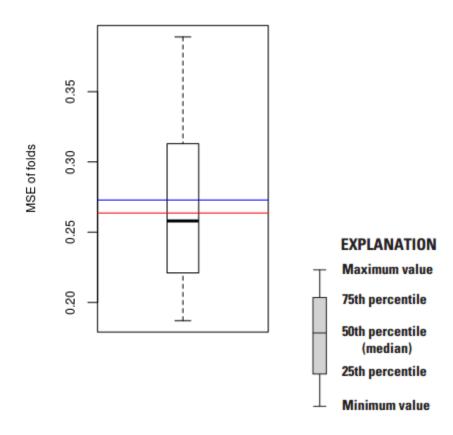
Fold - equal partition of the data (10 percent of the data).

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.

Minimum MSE of folds: 0.187
Mean MSE of folds: 0.273
Median MSE of folds: 0.258
Maximum MSE of folds: 0.389
(Mean MSE of folds) / (Model MSE): 1.040



Red line - Model MSE

Blue line - Mean MSE of folds

Model-Calibration Dataset

Model-Calibration Dataset											
	Date	logECB	logTBY	ECB	TBY	Computed	Computed	Residual	Normal	Censored	
0						logECB	ECB		Quantiles	Values	
1	2013-09-23	1.72	1.45	52	28	1.53	64.4	0.186	0.343		
2	2013-10-21	1.7	1.41	50	26	1.49	58.6	0.21	0.412		
3	2013-11-18	1.59	1.45	39	28.2	1.53	64.9	0.0571	0.21		
4	2013-12-16	0.477	1.36	3	23.1	1.42	50.4	-0.947	-1.68		
5	2014-01-13	1.18	1.15	15	14.2	1.16	27.2	0.0198	0.145		
6	2014-02-10	1.41	0.982	26	9.6	0.941	16.6	0.474	0.939		
7	2014-03-10	1.3	0.945	20	8.81	0.893	14.9	0.408	0.755		
8	2014-04-07	0.845	1.04	7	10.9	1.01	19.5	-0.166	-0.377		
9	2014-05-05	2.18	1.67	150	46.6	1.81	123	0.366	0.633		
10	2014-06-02	2.83	1.94	670	87.1	2.15	271	0.671	1.23		
11	2014-06-11	3.3	2.28	2000	190	2.58	729	0.717	1.3		
12	2014-06-30	1.95	1.7	90	50.2	1.85	135	0.103	0.276		
13	2014-07-14	1.48	1.59	30	39	1.71	98	-0.235	-0.556		
14	2014-07-28	1.52	1.36	33	23	1.42	50.2	0.0968	0.243		
15	2014-08-11	2.78	1.57	600	37	1.68	91.6	1.09	2.42		
16	2014-08-25	1.85	1.72	70	52	1.87	141	-0.0257	0.016		
17	2014-09-08	1.81	1.93	64	86	2.15	267	-0.342	-0.672		
18	2014-09-22	2.08	1.9	120	80.3	2.11	245	-0.031	-0.016		
19	2014-10-06	1.52	2.28	33	190	2.58	729	-1.07	-2.04		
20	2014-10-20	1.97	1.83	93	67	2.01	194	-0.0418	-0.0481		

21 2014-11-17	1.15	1.61	14 40.		102	-0.586	-1.16	
22 2014-12-15	1.56	1.58		8 1.7	94.8	-0.142	-0.276	
23 2015-01-12	1.36	0.971	23 9.3		16	0.435	0.89	
24 2015-02-09	1.2	1		0.963	17.5	0.241	0.483	
25 2015-03-09	0.903	0.97	8 9.3		16	-0.0222	0.0481	
26 2015-04-06	1.3	0.87	20 7.4		12	0.502	0.99	
27 2015-05-04	1.54	1.79		2 1.97	176	-0.424	-0.799	
28 2015-05-18	2.62	2.47	420 29		1270	-0.203	-0.519	
29 2015-06-01	2.51	2.36	320 23		929	-0.184	-0.483	
30 2015-06-15	2.11	2.25	130 18		678	-0.439	-0.843	
31 2015-06-29	1.69	2.26	49 18		681	-0.864	-1.46	
32 2015-07-13	1.89	2.08	77 12		407	-0.445	-0.89	
33 2015-07-27	2.04	1.64		4 1.78	114	0.263	0.556	
34 2015-08-10	2.76	1.94		8 2.16	275	0.603	1.1	
35 2015-08-24	1.89	1.7		0 1.85	134	0.0373	0.177	
36 2015-09-08	1.66	1.54		5 1.65	85.4	0.00992	0.0802	
37 2015-09-21	1.64	1.34		2 1.4	47.4	0.246	0.519	
38 2015-10-05	1.51	1.26	32 18.		37.5	0.209	0.377	
39 2015-10-19	1.67	1.26		8 1.29	36.8	0.385	0.672	
40 2015-11-16	1.58	1.15		4 1.15	26.7	0.431	0.843	
41 2015-12-14	3.9	2.75	7900 55		2850	0.722	1.38	
42 2016-01-11	1	1.61		1 1.74	104	-0.74	-1.38	
43 2016-02-08	0.954	1.36		3 1.42	50.2	-0.467	-1.04	
44 2016-03-03	0.903	1.15		4 1.15	26.7	-0.245	-0.594	
45 2016-04-04	1.15	1.04		1 1.02	19.7	0.13	0.309	
46 2016-05-02	3.51	2.51	3200 32		1410	0.634	1.16	
47 2016-05-16	2.4	2.27	250 18		721	-0.181	-0.447	
48 2016-06-06	1.83	1.96	68 91.		288	-0.348	-0.713	
49 2016-06-20	1.59	1.78	39 59.		168	-0.355	-0.755	
50 2016-07-11	1.85	1.76		8 1.93	162	-0.0858	-0.112	
51 2016-07-25	1.51	1.55	32 35.		86.4	-0.153	-0.309	
52 2016-08-08	2.86	2.32	730 21		828	0.224	0.447	
53 2016-08-22	3.3	2.2	2000 16		586	0.812	1.46	
54 2016-09-12	2.36	2.51	230 32		1430	-0.515	-1.1	
55 2016-09-26	3.36	2.18	2300 15		540	0.908	1.84	
56 2016-10-11	2.83	1.81		5 1.99	187	0.832	1.56	
57 2016-10-24	1.85	1.38		4 1.45	52.9	0.4	0.713	
58 2016-11-07	1.69	1.3		0 1.34	42	0.345	0.594	
59 2016-12-12	1.48	1.47	30 29.		69.3	-0.0847	-0.0802	
60 2017-01-09	0.699	1.01	5 10.		17.9	-0.275	-0.633	
61 2017-02-06	0.778	1.36		3 1.42	50.2	-0.644	-1.23	
62 2017-03-06	0.845	1.45	7 28.			-0.691	-1.3	
63 2017-04-10	2.11	1.98		6 2.21	307	-0.0943	-0.145	
64 2017-05-08	1.99	1.94	97 86.		270	-0.165	-0.343	
65 2017-05-22	3.57	2.62	3700 42		1990	0.547	1.04	
66 2017-06-05	1.99	2.18	97 15		540	-0.467	-0.99	
67 2017-06-19	1.95	1.87		4 2.06	221	-0.111	-0.21	
68 2018-10-11	3.91	2.65	8200 45		2180	0.855	1.68	
69 2018-11-28	1.4	1.7	25 50.		135	-0.452	-0.939	
70 2018-12-17	1.11	2.01	13 10		333	-1.13	-2.42	
71 2019-02-05	1.92	1.74	83 54.		151	0.0191	0.112	
72 2019-03-18	2.15	2.75	140 55		2850	-1.03	-1.84	
73 2019-04-15	1.18	1.89	15 76.		232	-0.91	-1.56	
74 2019-05-09	4.26		18000 55		2830	1.08	2.04	
75 2019-06-25	3.36	2.56	2300 36	7 2.95	1680	0.416	0.799	

76 2019-07-15	1.66	1.63	46 42.7	1.76	110	-0.0991	-0.177	
77 2019-08-19	2.04	1.94	110 87.3	2.16	272	-0.115	-0.243	
78 2019-09-23	2.28	2.17	190 149	2.45	536	-0.172	-0.412	

Definitions

Cook's D: Cook's distance (Helsel and others, 2020).

DFFITS: Difference in fits statistic (Helsel and others, 2020).

E.vars: Explanatory variables.

ECB: Escherichia coli, in colonies per 100 milliliters (90902).

Leverage: An outlier's measure in the x direction (Helsel and others, 2020).

LOESS: Local polynomial regression fitting, or locally estimated scatterplot smoothing (Helsel and others, 2020).

LOWESS: Locally weighted scatterplot smoothing (Cleveland, 1979; Helsel and others, 2020).

MSE: Model standard error (Helsel and others, 2020).

MSPE: Model standard percentage error (Helsel and others, 2020).

Probability(>|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).

t value: Student's t value; the coefficient divided by its associated standard error (Helsel and others, 2020).

TBY: Turbidity, in formazin nephelometric units (63680).

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