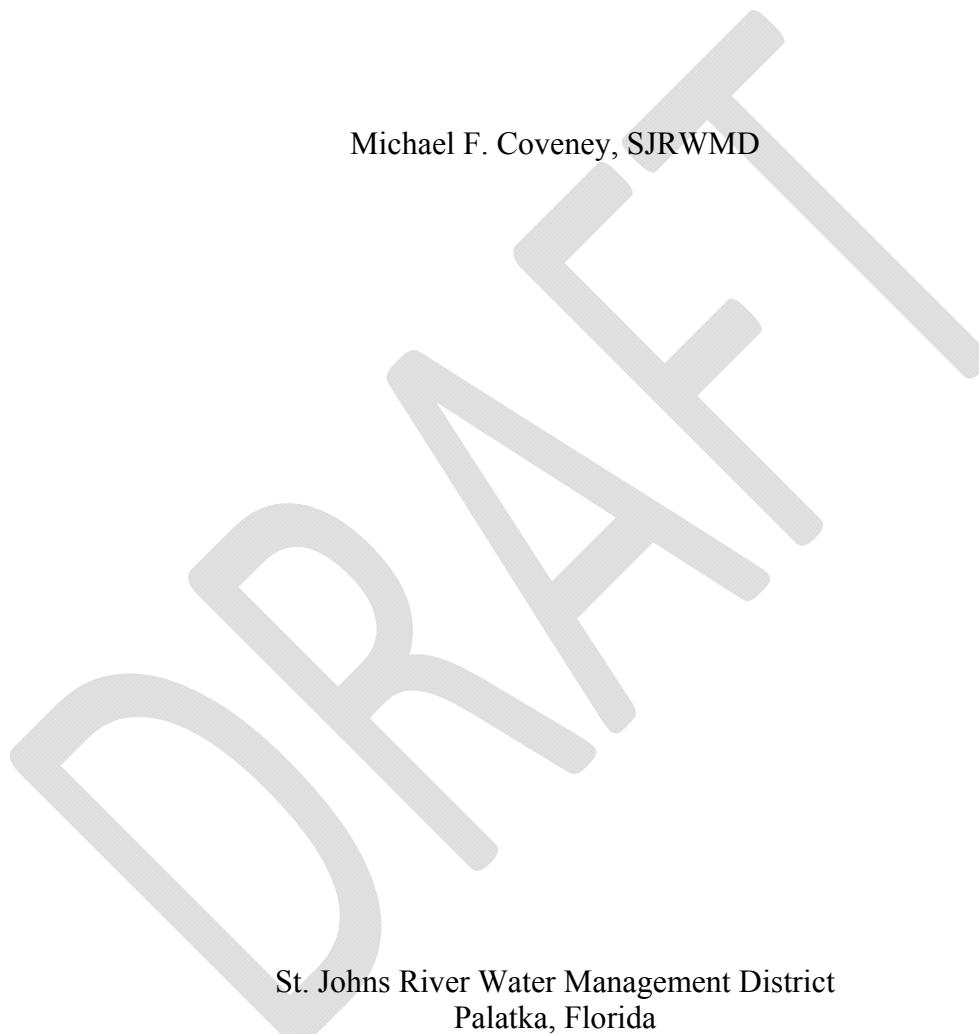


Appendix 8.C. Empirical Regression Models and Goodness-of-Fit Diagnostics

Michael F. Coveney, SJRWMD



St. Johns River Water Management District
Palatka, Florida
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Introduction

The St. Johns River Water Management District's Water Supply Impact Study evaluated potential effects of water supply withdrawals from the St. Johns River (SJR) on biological and water resources. The Plankton Working Group was charged with the identification and quantification of possible environmental effects of water withdrawals on plankton communities and Total Maximum Daily Loads. Most of the potential effects that we investigated were causes or consequences of enhanced growth of phytoplankton. Consequently, phytoplankton blooms, primarily cyanobacteria in fresh water and dinoflagellates in brackish water, were a primary focus of our work. One important step in this work was to develop hydroecological regression models that link changes in hydrology to changes in plankton communities.

We aggregated the effects of algal blooms into four algal bloom metrics: marine algal blooms (dinoflagellate biovolume), increase in nitrogen (N) load due to N₂-fixation, magnitude of freshwater algal blooms (maximum chlorophyll-a concentration), and duration of freshwater algal blooms. We used water age (a measure of residence time) as the primary hydrologic variable and constructed empirical regression models to relate algal bloom metrics to water age variables. Water age was calculated in the Environmental Fluids Dynamic Code (EFDC) hydrodynamic model and was the average time that water resided in the model domain before reaching a specific site (model grid cell).

We constructed a total of eight regression models using both multiple linear and multiple logistic regression techniques (Table 1). These regression models covered the four algal bloom metrics in four of the five river segments that we assessed (Lake Poinsett in segment 8 was assessed separately; see Appendix 8.B.). Seven of the regression models were linear regressions with adjusted R² values that varied from 0.80 to 0.97. In each case, both the overall model and the individual independent variables were significant ($p < 0.05$). The remaining model, freshwater bloom duration in segments 3 and 4, was a logistic regression with two independent variables. In this case, we chose logistic regression because the best-fit linear regression model achieved only a modest R² value. Regression models were constructed using either stepwise (forward and backward selection) or R² selection of independent variables for linear regression and by highest likelihood score selection for logistic regression. SAS[®] was used in these analyses.

We assessed potential effects of water withdrawals by using the empirical regression models to predict algal bloom measures from water age variables. We used water age output from the EFDC hydrodynamic model for the baseline scenario and each withdrawal scenario and compared the predicted bloom measures. By focusing on the difference between predicted results for the baseline scenario and for withdrawal scenarios, we minimized effects of model bias since the bias would be present in both sets of results.

Dependent and Independent Variables

Dependent variables for regression models were the quantities measured for each of the four algal bloom metrics (Table 1). These variables were tabulated annually and represented either the maximum (biovolume, chl-a, bloom duration) or the total (mass N₂-fixation) for each year. No variables were transformed except for maximum annual dinoflagellate biovolume, where logarithmic transformation appeared to be necessary (Chapter 8. Plankton).

Table 1. Regression type, source location(s) for data, and dependent variable names used in each regression model. See Chapter 8. Plankton for sampling sites corresponding to these locations.

Bloom Measure	Segment	Type	Data Source Location	Dependent Variable
ln(Dinoflag Biovolume)	2	Linear	Mandarin Pt Doctors Lake	LNMaxDino
N ₂ -Fixation	3,4	Linear	Lake George	Est_N2_Fix
FW Max Chl-a	2	Linear	Doctors Lake	Max_Chla
FW Max Chl-a	3,4	Linear	Racy Pt Lake George	Max_Chla
FW Max Chl-a	6	Linear	Lake Monroe Lake Jesup Lake Harney	Max_Chla
FW Bloom Duration	2	Linear	Doctors Lake	Longest_d
FW Bloom Duration Event	3,4	Logistic	Racy Pt Palatka Lake George	Bloom_50d
FW Bloom Duration	6	Linear	Lake Monroe Lake Jesup	Longest_dur_Bloom

Independent variables for regression models were minimum, mean, and maximum daily water age and the inverse of each water age calculated for seven periods, for a total of 42 possible variables (Table 2). Time periods were five quarters (A – E, starting with the last quarter of the previous calendar year) and two growth-season periods (Apr – Aug and Apr – Oct) (Table 2).

Appendix 8.C.

We included this wide range of water age variables as potential prediction variables in regression models because relationships between algal bloom patterns and hydrology were both positive and negative and showed complex seasonality (Chapter 8. Plankton).

The period for observed data used to build regression models was determined by the eleven-year simulation period for the hydrodynamic model: January 1995 through December 2005. Because model initiation (“spin-up”) caused low water age values during the first three months, we did not use data from Jan – March 1995.

Table 2. Naming convention for water age (independent) variables. Variable names were combinations of two forms (value, inverse value), three statistics (mean, minimum, maximum), and seven periods, for a total of 42 variables. Examples of water age variables using this convention were MeanAgeD (mean daily water age for period D), Min_Age_Apr_Oct (minimum daily water age for the period April – October), and invMaxAgeA (the inverse of the maximum daily water age for period A). Variable names varied slightly between analysts; e.g., both “mean” and “avg” were used for mean, and position of underscore characters differed.

Forms	Statistics	Periods
Water age value	Mean	April – October
Inverse of the water age value	Minimum	April – August
	Maximum	A (Oct-Dec of previous year) B (Jan-Mar) C (Apr-Jun) D (Jul-Sep) E (Oct-Dec)

SAS[®] Calculation of Regression Models

A. Dinoflagellate Biovolume, Segment 2

```

The REG Procedure
Model: MODEL1
Dependent Variable: LNMaxDino LNMaxDino

Number of Observations Read          20
Number of Observations Used         20

Analysis of Variance

Source           DF   Sum of Squares   Mean Square   F Value   Pr > F
Model            5    36.50278     7.30056      17.36    <.0001
Error            14   5.88607      0.42043
Corrected Total  19   42.38885

Root MSE        0.64841   R-Square       0.8611
Dependent Mean  5.39282   Adj R-Sq       0.8115
Coeff Var       12.02355

Parameter Estimates

Variable        Label   DF   Parameter Estimate   Standard Error   t Value   Pr > |t|
Intercept       Intercept 1    7.31406     2.06093      3.55    0.0032
Inv_Max_Age_E  Inv_Max_Age_E 1   390.31362    124.20677    3.14    0.0072
Inv_Min_Age_D  Inv_Min_Age_D 1  -540.09679    147.07539   -3.67    0.0025
Max_Apr_Oct    Max_Apr_Oct  1   0.15035     0.02471      6.08    <.0001
Max_Age_C       Max_Age_C   1   -0.12813     0.02268    -5.65    <.0001
Min_Age_D       Min_Age_D   1   -0.04082     0.01245    -3.28    0.0055

Parameter Estimates

Variable        Label   DF   Standardized Estimate
Intercept       Intercept 1      0
Inv_Max_Age_E  Inv_Max_Age_E 1   0.80224
Inv_Min_Age_D  Inv_Min_Age_D 1  -1.47481
Max_Apr_Oct    Max_Apr_Oct  1   6.30995
Max_Age_C       Max_Age_C   1  -5.05773
Min_Age_D       Min_Age_D   1  -1.49375

```

Appendix 8.C.

B. N₂-Fixation, Segments 3 & 4

```

The REG Procedure
      Model: MODEL1
      Dependent Variable: Est_N2_Fix Est_N2_Fix

Number of Observations Read                      22
Number of Observations Used                     10
Number of Observations with Missing Values     12

Analysis of Variance

Source          DF   Sum of Squares   Mean Square   F Value   Pr > F
Model            3       3689415      1229805      76.29    <.0001
Error            6        96722       16120
Corrected Total  9       3786137

Root MSE        126.96616   R-Square       0.9745
Dependent Mean  806.26123   Adj R-Sq       0.9617
Coeff Var       15.74752

Parameter Estimates

Variable        Label      DF   Parameter Estimate   Standard Error   t Value   Pr > |t|
Intercept       Intercept  1       444.94101   213.20432      2.09    0.0819
MeanAgeD        MeanAgeD  1       4.67005     1.15732      4.04    0.0068
invMeanAgeB     invMeanAgeB 1      -259099     21012      -12.33    <.0001
invMinAgeC      invMinAgeC 1       242239      16316      14.85    <.0001

Parameter Estimates

Variable        Label      DF   Standardized Estimate
Intercept       Intercept  1           0
MeanAgeD        MeanAgeD  1       0.29719
invMeanAgeB     invMeanAgeB 1      -2.16507
invMinAgeC      invMinAgeC 1       2.63640

```

Appendix 8.C.

C. Freshwater Maximum Chl-a, Segment 2

```

The REG Procedure
Model: MODEL1
Dependent Variable: Max_Ch1 Max_Ch1

Number of Observations Read                      11
Number of Observations Used                     10
Number of Observations with Missing Values      1

Analysis of Variance

Source          DF   Sum of Squares   Mean Square   F Value   Pr > F
Model           4    10217        2554.17668    23.64     0.0019
Error           5    540.17729      108.03546
Corrected Total 9    10757

Root MSE       10.39401   R-Square       0.9498
Dependent Mean 82.34000   Adj R-Sq       0.9096
Coeff Var      12.62328

Parameter Estimates

Variable       Label       DF   Parameter Estimate   Standard Error   t Value   Pr > |t|
Intercept     Intercept   1    100.21543    39.22541      2.55     0.0510
Ave_Apr_Aug   Ave_Apr_Aug 1    3.62191     0.43635      8.30     0.0004
Inv_Ave_Age_A Inv_Ave_Age_A 1    57722        20280      2.85     0.0360
Inv_Max_Age_A Inv_Max_Age_A 1    -65902       20501     -3.21     0.0236
Max_Apr_Oct   Max_Apr_Oct  1    -3.16151     0.40773     -7.75     0.0006

Parameter Estimates

Variable       Label       DF   Standardized Estimate
Intercept     Intercept   1    0
Ave_Apr_Aug   Ave_Apr_Aug 1    5.89187
Inv_Ave_Age_A Inv_Ave_Age_A 1    2.44664
Inv_Max_Age_A Inv_Max_Age_A 1    -2.73423
Max_Apr_Oct   Max_Apr_Oct  1    -5.57109

```

Appendix 8.C.

D. Freshwater Maximum Chl-a, Segments 3 & 4

The REG Procedure Model: MODEL1 Dependent Variable: Max_Ch1 Max_Ch1					
Number of Observations Read				22	
Number of Observations Used				20	
Number of Observations with Missing Values				2	
Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	7	18074	2582.06611	21.60	<.0001
Error	12	1434.20270	119.51689		
Corrected Total	19	19509			
Root MSE		10.93238	R-Square	0.9265	
Dependent Mean		94.16500	Adj R-Sq	0.8836	
Coeff Var		11.60981			
Parameter Estimates					
Variable	Label	DF	Parameter Estimate	Standard Error	t Value
Intercept	Intercept	1	24.63329	71.77171	0.34
MeanAgeD	MeanAgeD	1	1.00042	0.28955	3.46
MinAgeD	MinAgeD	1	-2.36030	0.29282	-8.06
MaxAgeE	MaxAgeE	1	0.86558	0.14935	5.80
invMean_Age_Apr_Oct	invMean_Age_Apr_Oct	1	6121.89276	2507.95714	2.44
invMeanAgeE	invMeanAgeE	1	3916.79838	965.69610	4.06
invMinAgeD	invMinAgeD	1	-7892.28591	1238.47933	-6.37
invMaxAgeA	invMaxAgeA	1	3676.65842	1016.17188	3.62
Parameter Estimates					
Variable	Label	DF	Pr > t	Standardized Estimate	
Intercept	Intercept	1	0.7374	0	
MeanAgeD	MeanAgeD	1	0.0048	1.36713	
MinAgeD	MinAgeD	1	<.0001	-2.31831	
MaxAgeE	MaxAgeE	1	<.0001	1.29710	
invMean_Age_Apr_Oct	invMean_Age_Apr_Oct	1	0.0311	0.63618	
invMeanAgeE	invMeanAgeE	1	0.0016	0.75460	
invMinAgeD	invMinAgeD	1	<.0001	-1.76370	
invMaxAgeA	invMaxAgeA	1	0.0035	0.54011	

Appendix 8.C.

E. Freshwater Maximum Chl-a, Segment 6

The REG Procedure						
Model: MODEL1						
Dependent Variable: Max_Chla Max_Chla						
Number of Observations Read			33			
Number of Observations Used			30			
Number of Observations with Missing Values			3			
Analysis of Variance						
Source	DF	Sum of Squares	Mean Square	F Value	Pr > F	
Model	4	130729	32682	30.41	<.0001	
Error	25	26871	1074.85196			
Corrected Total	29	157600				
Root MSE		32.78494	R-Square	0.8295		
Dependent Mean		93.98230	Adj R-Sq	0.8022		
Coeff Var		34.88416				
Parameter Estimates						
Variable	Label	DF	Parameter Estimate	Standard Error	t Value	Pr > t
Intercept	Intercept	1	4.04120	10.67110	0.38	0.7081
Min_Apr_Oct	Min_Apr_Oct	1	-4.81072	1.38030	-3.49	0.0018
Max_Age_B	Max_Age_B	1	0.73032	0.17495	4.17	0.0003
Min_Age_D	Min_Age_D	1	2.15419	0.65338	3.30	0.0029
Min_Age_E	Min_Age_E	1	3.43669	1.07992	3.18	0.0039
Parameter Estimates						
Variable	Label	DF	Standardized Estimate			
Intercept	Intercept	1	0			
Min_Apr_Oct	Min_Apr_Oct	1	-1.79980			
Max_Age_B	Max_Age_B	1	0.50293			
Min_Age_D	Min_Age_D	1	0.90130			
Min_Age_E	Min_Age_E	1	1.33638			

Appendix 8.C.

F. Freshwater Bloom Duration, Segment 2

```

The REG Procedure
Model: MODEL1
Dependent Variable: Longest_d Longest_d

Number of Observations Read                      11
Number of Observations Used                     10
Number of Observations with Missing Values      1

Analysis of Variance

Source          DF   Sum of Squares   Mean Square   F Value   Pr > F
Model           4    23431        5857.75456    63.87    0.0002
Error           5    458.58175     91.71635
Corrected Total 9    23890

Root MSE       9.57687   R-Square       0.9808
Dependent Mean 103.80000  Adj R-Sq       0.9654
Coeff Var      9.22627

Parameter Estimates

Variable        Label          DF   Parameter Estimate   Standard Error   t Value
Intercept       Intercept      1    538.44157    44.83292    12.01
Ave_Age_A       Ave_Age_A     1    -1.90085    1.06921    -1.78
Ave_Age_D       Ave_Age_D     1    -2.34085    0.19796    -11.83
Inv_Min_Apr_Oct Inv_Min_Apr_Oct 1    -31891      3700.23837   -8.62
Max_Age_A       Max_Age_A     1    3.13881     0.85479    3.67

Parameter Estimates

Variable        Label          DF   Pr > |t|   Standardized Estimate
Intercept       Intercept      1    <.0001      0
Ave_Age_A       Ave_Age_A     1    0.1356    -1.39338
Ave_Age_D       Ave_Age_D     1    <.0001    -2.57233
Inv_Min_Apr_Oct Inv_Min_Apr_Oct 1    0.0003    -1.36967
Max_Age_A       Max_Age_A     1    0.0144    2.70134

```

Appendix 8.C.

G. Freshwater Bloom Duration, Segments 3 & 4

The LOGISTIC Procedure

Model Information

Data Set	WORK.TEMP	
Response Variable	Bloom_50d	Bloom_50d
Number of Response Levels	2	
Model	binary logit	
Optimization Technique	Fisher's scoring	

Number of Observations Read	39
Number of Observations Used	33

Response Profile

Ordered Value	Bloom_50d	Total Frequency
1	0	14
2	1	19

Probability modeled is Bloom_50d=1.

NOTE: 6 observations were deleted due to missing values for the response or explanatory variables.

Model Convergence Status

Convergence criterion (GCONV=1E-8) satisfied.

Model Fit Statistics

Criterion	Intercept Only	Intercept and Covariates
AIC	46.987	33.008
SC	48.484	37.497
-2 Log L	44.987	27.008

R-Square 0.4201 Max-rescaled R-Square 0.5645

Testing Global Null Hypothesis: BETA=0

Test	Chi-Square	DF	Pr > ChiSq
Likelihood Ratio	17.9794	2	0.0001
Score	13.3032	2	0.0013
Wald	7.2636	2	0.0265

Appendix 8.C.

Analysis of Maximum Likelihood Estimates

Parameter	DF	Estimate	Standard Error	Chi-Square	Pr > ChiSq
Intercept	1	-26.4944	9.9179	7.1362	0.0076
Mean_Age_Apr_Aug	1	0.1331	0.0494	7.2606	0.0070
invMeanAgeC	1	1155.3	448.4	6.6378	0.0100

Odds Ratio Estimates

Effect	Point Estimate	95% Confidence Limits	Wald
Mean_Age_Apr_Aug	1.142	1.037	1.258
invMeanAgeC	>999.999	>999.999	>999.999

Association of Predicted Probabilities and Observed Responses

Percent Concordant	91.0	Somers' D	0.823
Percent Discordant	8.6	Gamma	0.826
Percent Tied	0.4	Tau-a	0.415
Pairs	266	c	0.912

Partition for the Hosmer and Lemeshow Test

Group	Total	Bloom_50d = 1		Bloom_50d = 0	
		Observed	Expected	Observed	Expected
1	3	1	0.14	2	2.86
2	3	0	0.44	3	2.56
3	3	0	0.79	3	2.21
4	3	0	1.13	3	1.87
5	3	1	1.31	2	1.69
6	3	3	1.65	0	1.35
7	3	3	2.18	0	0.82
8	3	2	2.58	1	0.42
9	3	3	2.81	0	0.19
10	3	3	2.96	0	0.04
11	3	3	2.99	0	0.01

Hosmer and Lemeshow Goodness-of-Fit Test

Chi-Square	DF	Pr > ChiSq
13.6939	9	0.1336

Appendix 8.C.

H. Freshwater Bloom Duration, Segment 6

The REG Procedure
 Model: MODEL1
 Dependent Variable: Longest_Dur_Bloom Longest_Dur_Bloom

Number of Observations Read	22
Number of Observations Used	20
Number of Observations with Missing Values	2

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	4	90152	22538	48.97	<.0001
Error	15	6903.94924	460.26328		
Corrected Total	19	97056			

Root MSE	21.45375	R-Square	0.9289
Dependent Mean	104.00000	Adj R-Sq	0.9099
Coeff Var	20.62860		

Parameter Estimates

Variable	Label	DF	Parameter Estimate	Standard Error	t Value
Intercept	Intercept	1	-44.37433	35.92549	-1.24
Inv_Ave_Apr_Oct	Inv_Ave_Apr_Oct	1	-7370.26368	1804.32954	-4.08
Inv_Max_Apr_Oct	Inv_Max_Apr_Oct	1	15172	3532.35554	4.30
Ave_Age_A	Ave_Age_A	1	0.51719	0.19136	2.70
Max_Age_D	Max_Age_D	1	0.95232	0.18157	5.25

Parameter Estimates

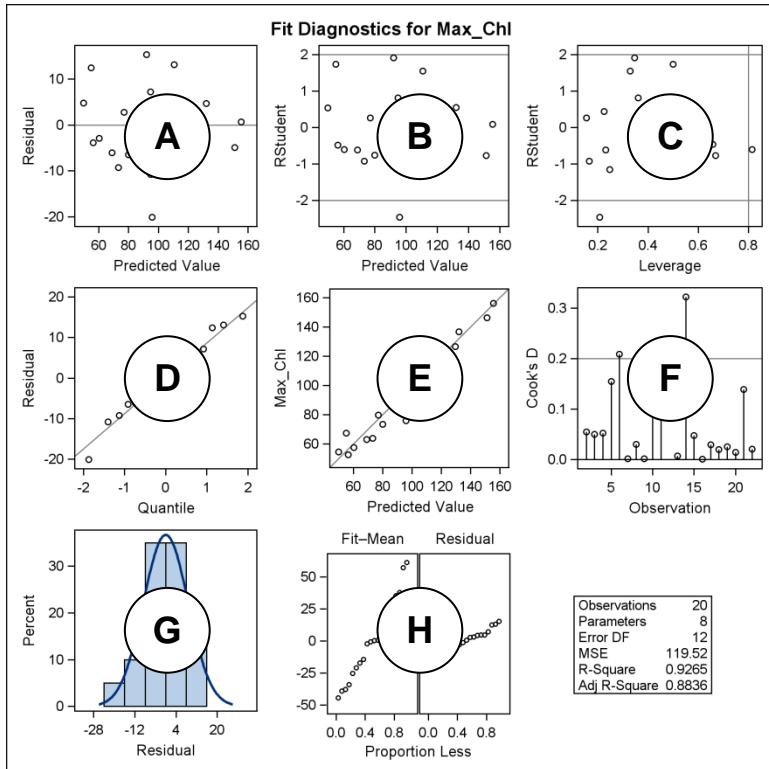
Variable	Label	DF	Pr > t	Standardized Estimate
Intercept	Intercept	1	0.2358	0
Inv_Ave_Apr_Oct	Inv_Ave_Apr_Oct	1	0.0010	-1.01649
Inv_Max_Apr_Oct	Inv_Max_Apr_Oct	1	0.0006	1.02284
Ave_Age_A	Ave_Age_A	1	0.0164	0.26288
Max_Age_D	Max_Age_D	1	<.0001	0.70370

SAS® Goodness-of-Fit Diagnostics for Regression Models

I. Introduction and Key

We show a set of diagnostic plots (SAS Institute Inc. 2010, page 6302) below for each of the seven linear regression models. Goodness-of-fit metrics for the logistic regression model (freshwater bloom duration, segments 3 & 4) are included in model calculation (above).

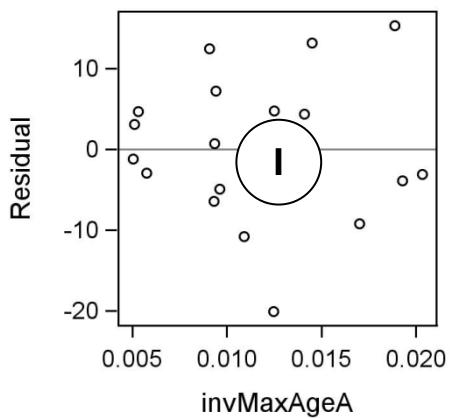
1. Key - Fit Diagnostic Plots



- Residuals vs predicted values
- Externally studentized residuals vs predicted values
- Externally studentized residuals vs leverage
- Normal quantile-quantile (Q-Q) plot of residuals
- Observed values vs predicted values
- Cook's D vs observation number
- Histogram of residuals
- Residual-Fit (RF): quantile plots of the centered fit and the residuals

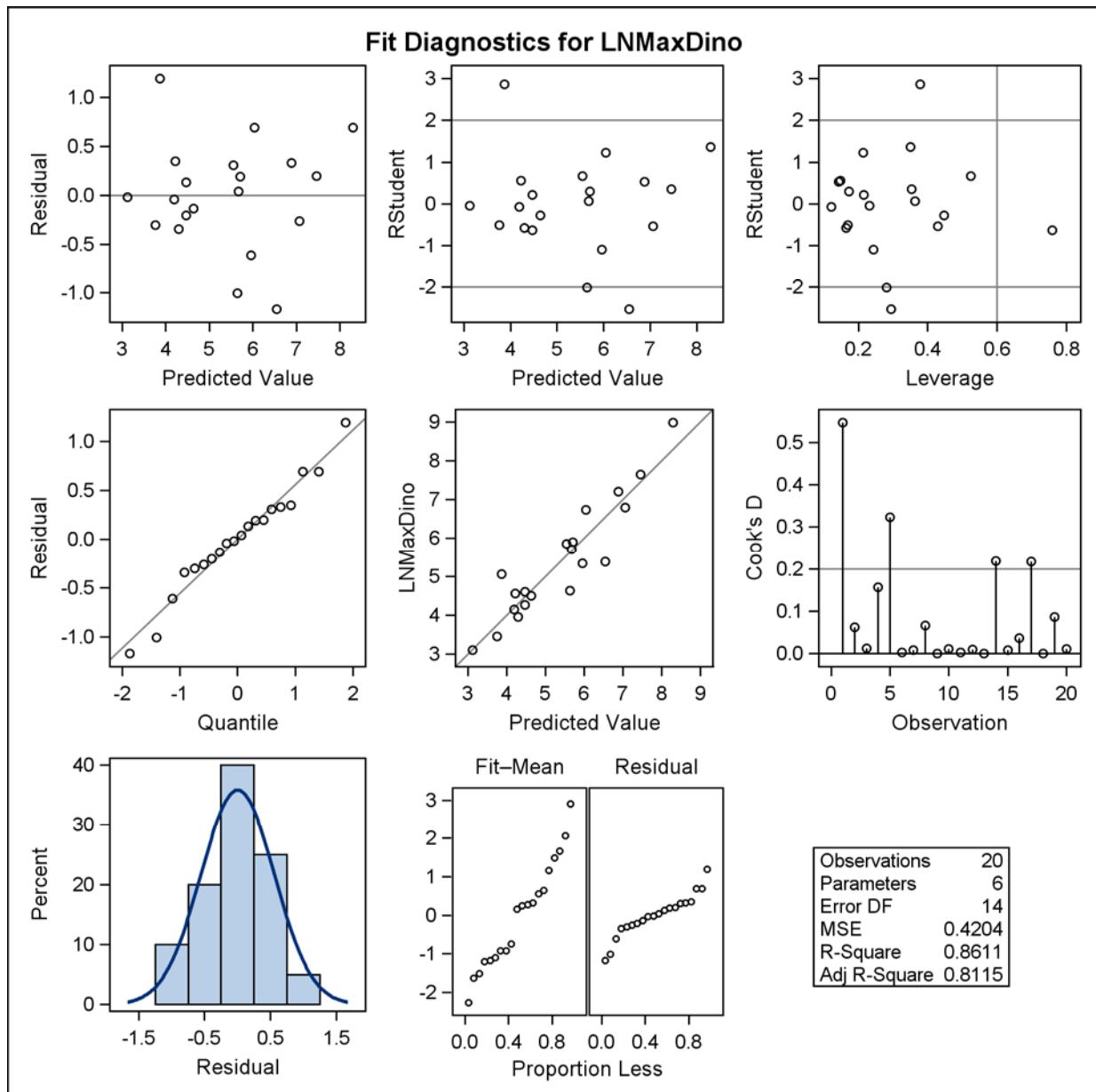
Plots A, B, and H help diagnose the adequacy of models. Better models lack patterns in the plots of residuals or studentized residuals versus predicted values (A, B), and the spread of residuals is less than the spread of the centered fit in the RF plot (H). Better models also lack patterns in the spread about the 1:1 reference line in the plot of observed values versus predicted values (E). The Q-Q plot (D) and residual histogram plot (G) can indicate problems with lack of normality and with heteroscedasticity. Plot B provides a test for outliers (defined as observations with studentized residuals greater than 2). Plots C and F identify observations with high leverage values (indicated by index lines). Further information is found in the SAS/STAT 9.22 User's Guide (SAS Institute Inc. 2010, page 6301-2).

2. Key - Residuals by Regressors (Independent Variables)

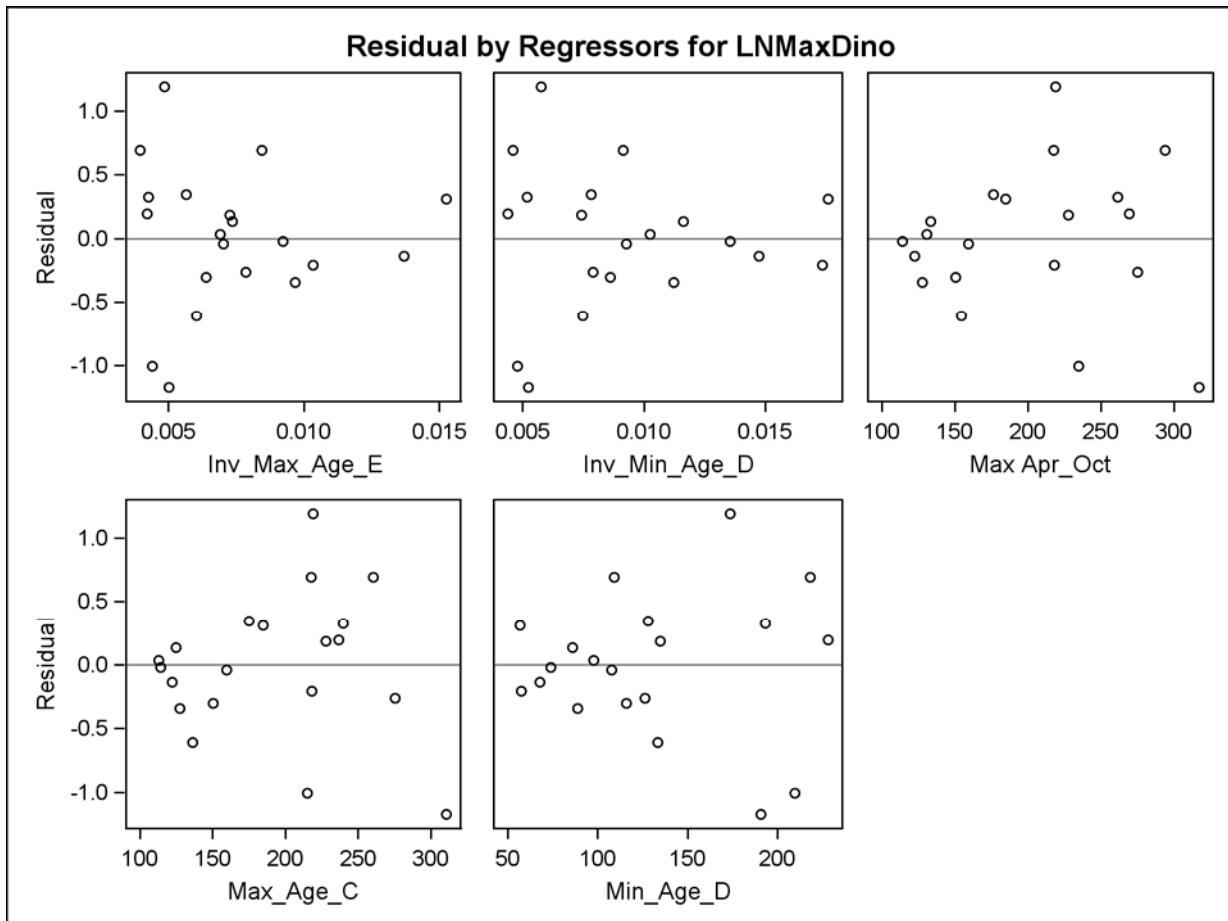


Plots of residuals vs each of the individual independent variables (I) also help to diagnose the adequacy of models; better models do not show patterns in these scatter plots. Further information is found in SAS/STAT 9.22 User's Guide (SAS Institute Inc. 2010, page 6302).

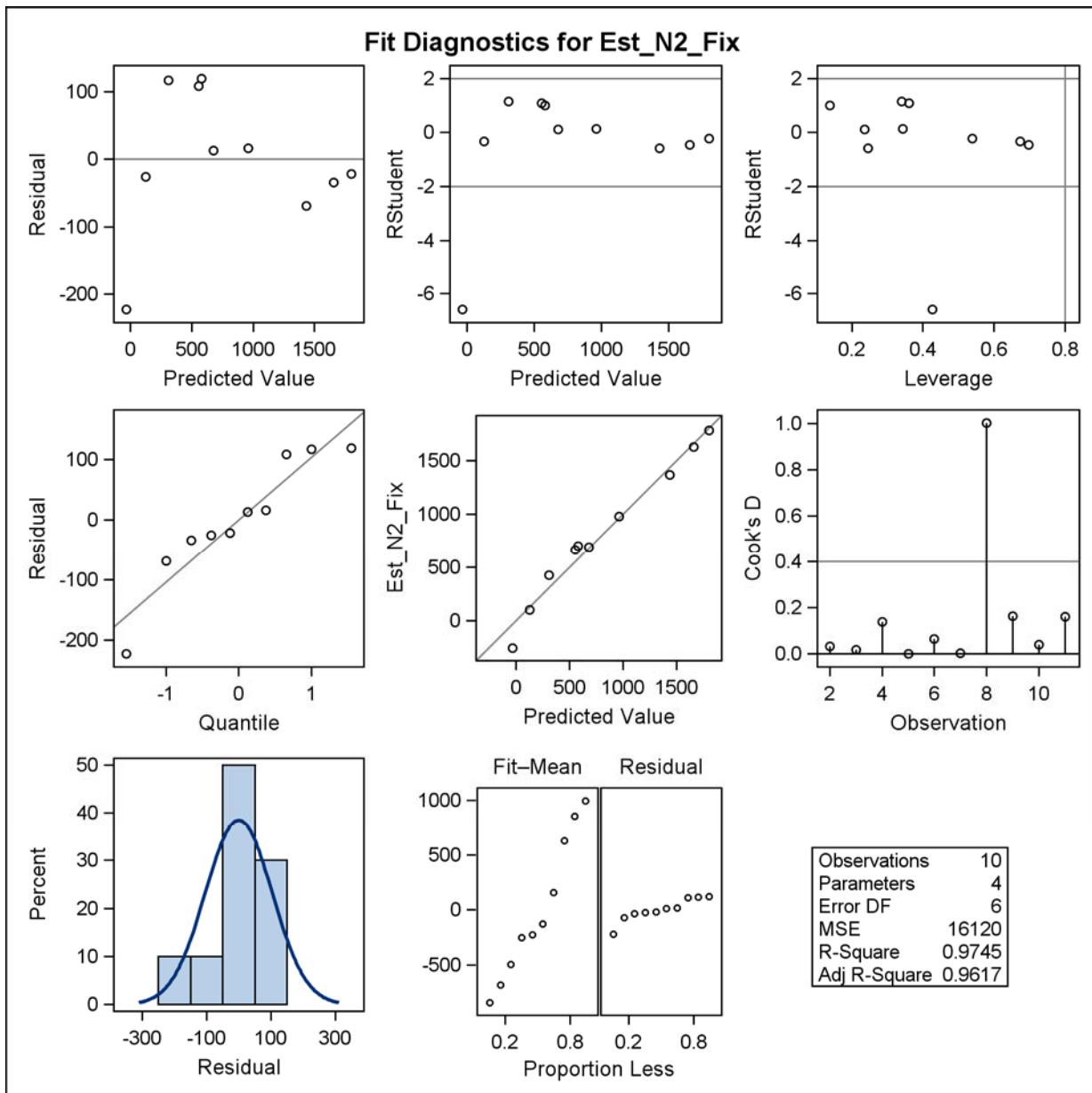
J. Dinoflagellate Biovolume, Segment 2



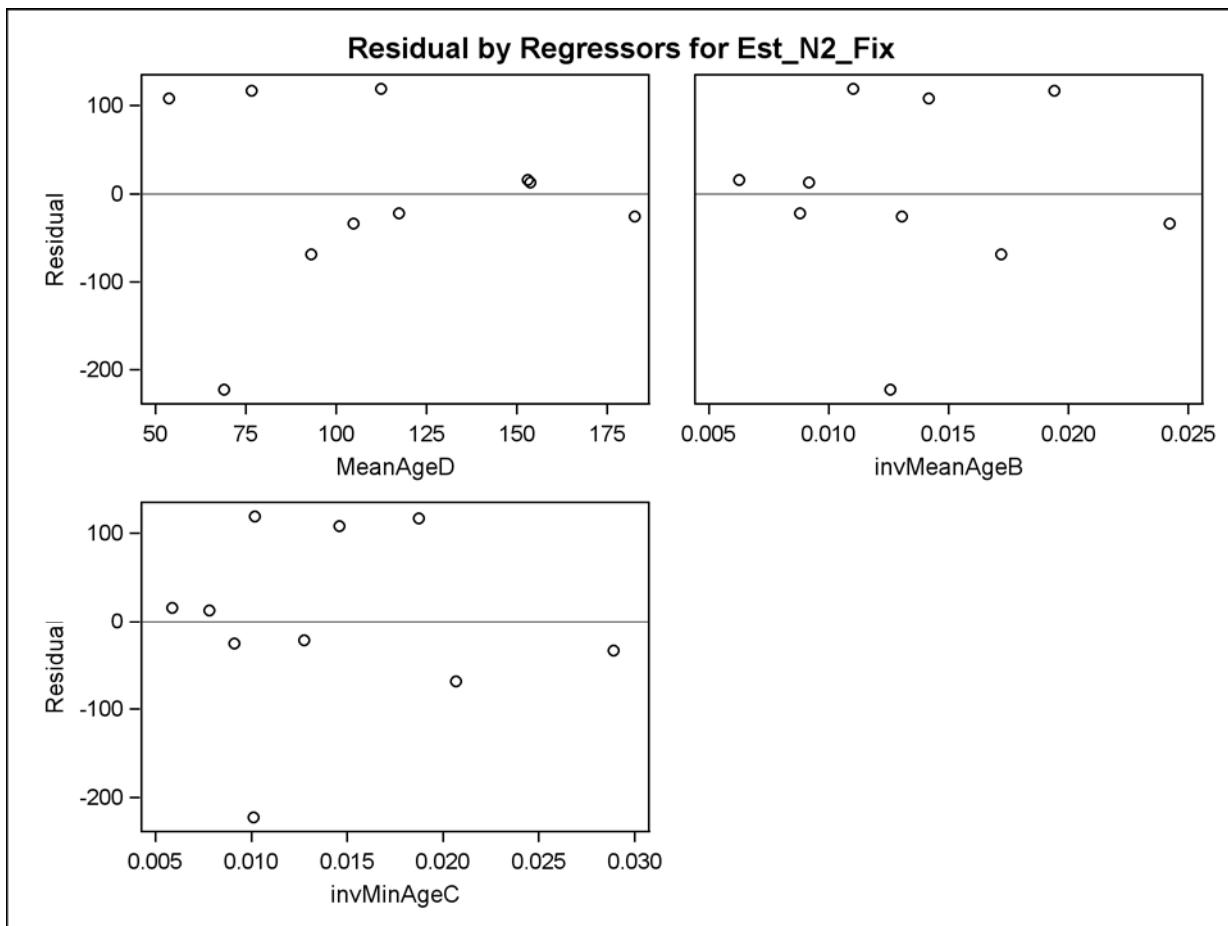
Appendix 8.C.



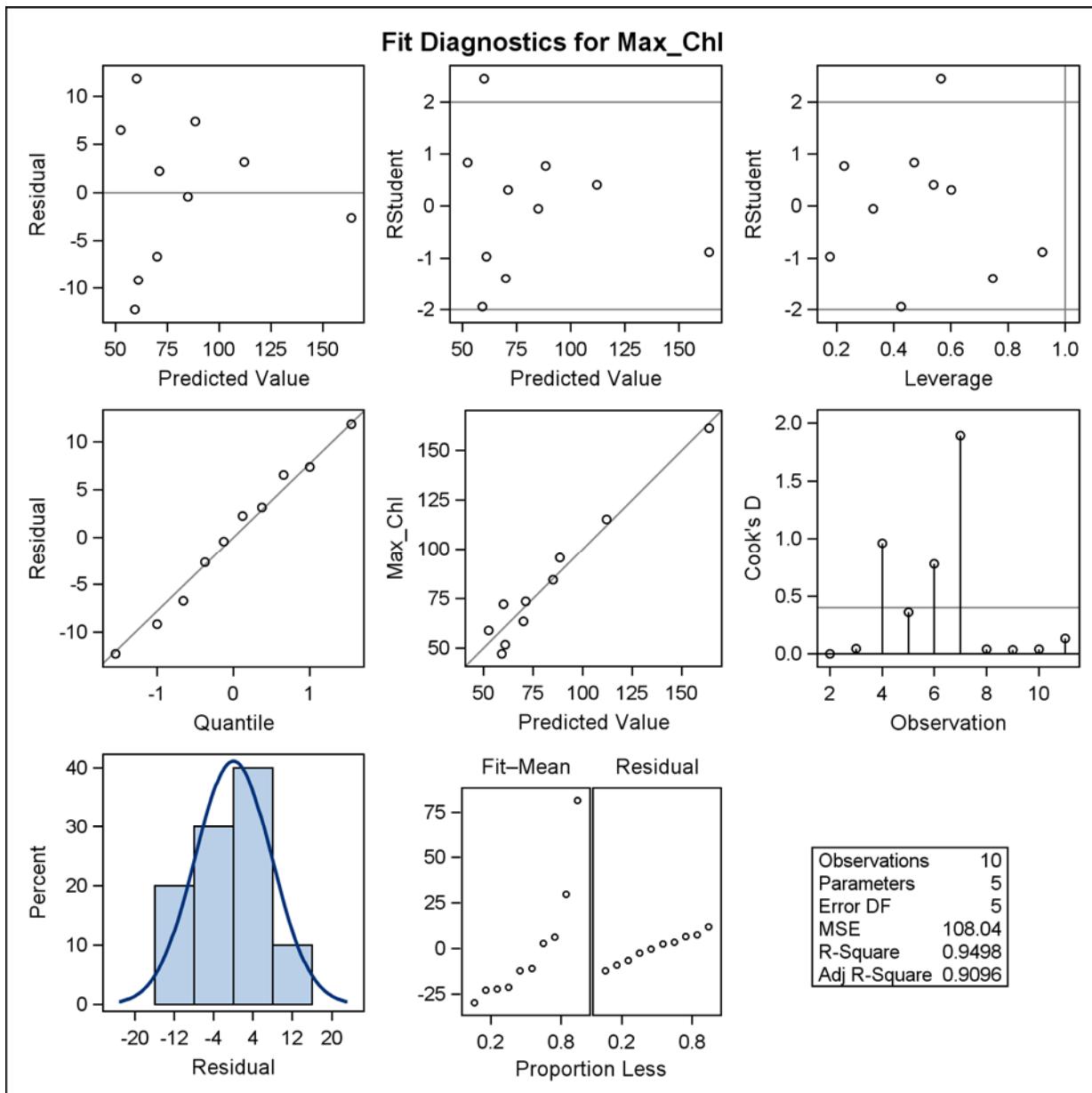
K. N₂-Fixation, Segments 3 & 4



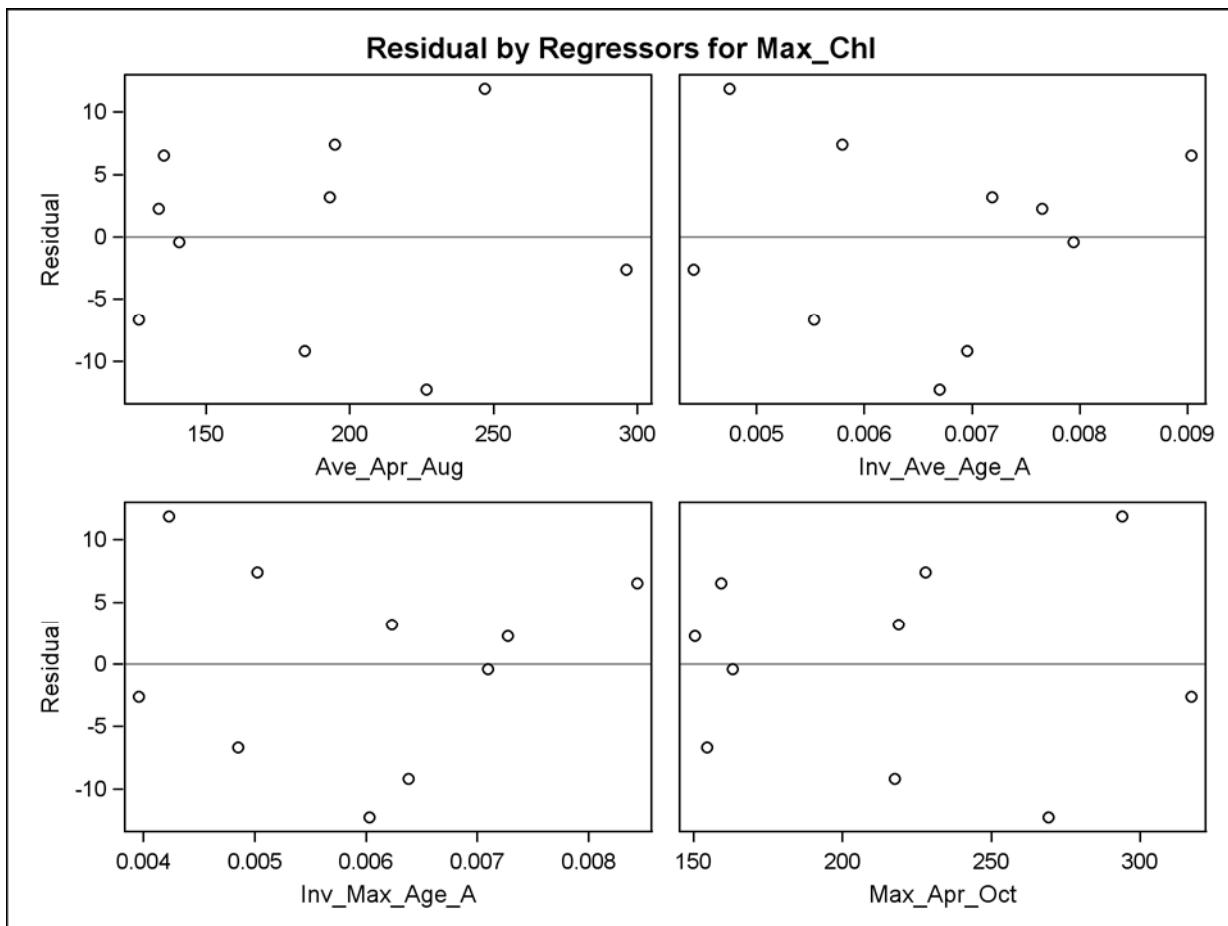
Appendix 8.C.



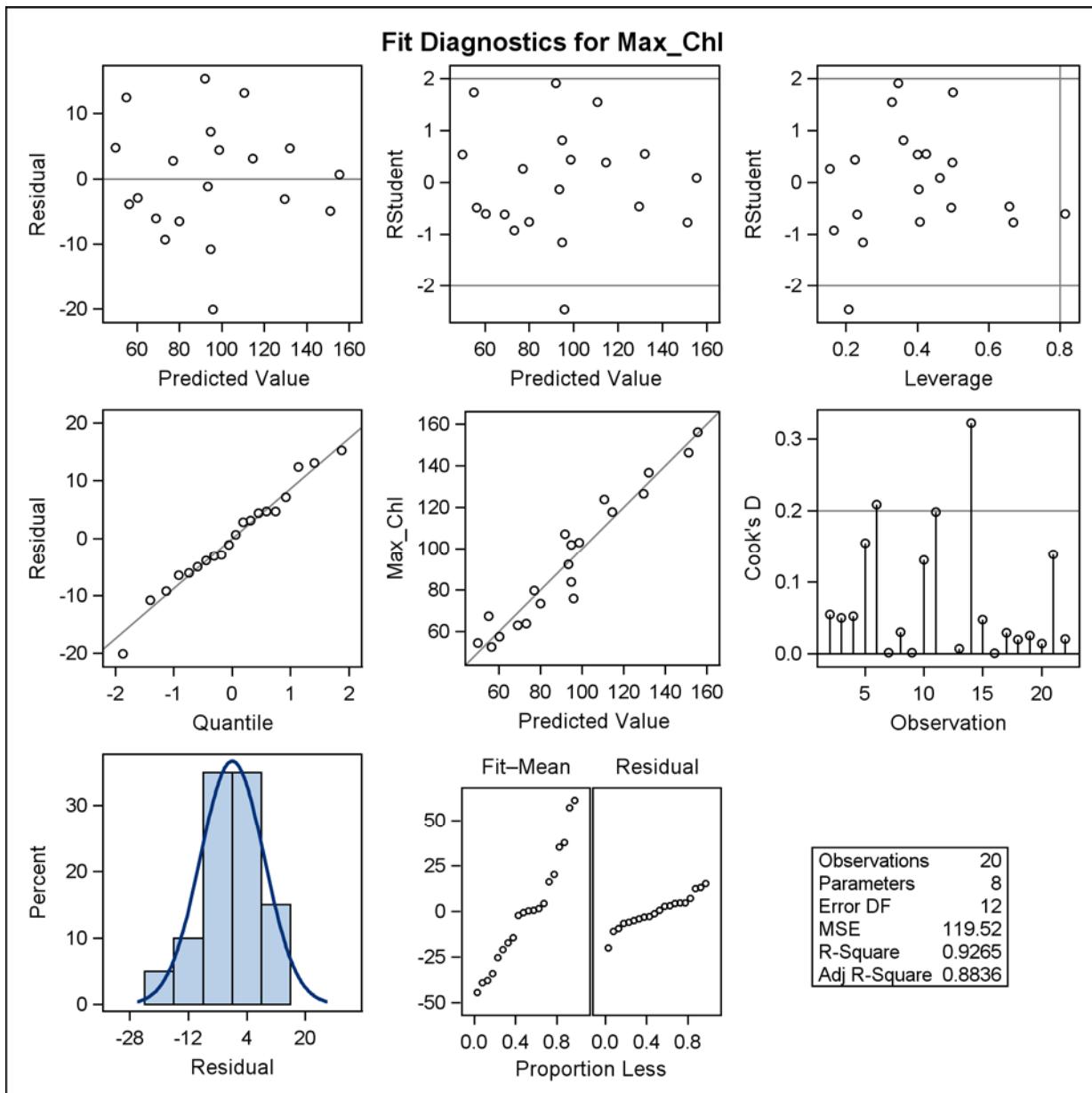
L. Freshwater Maximum Chl-a, Segment 2



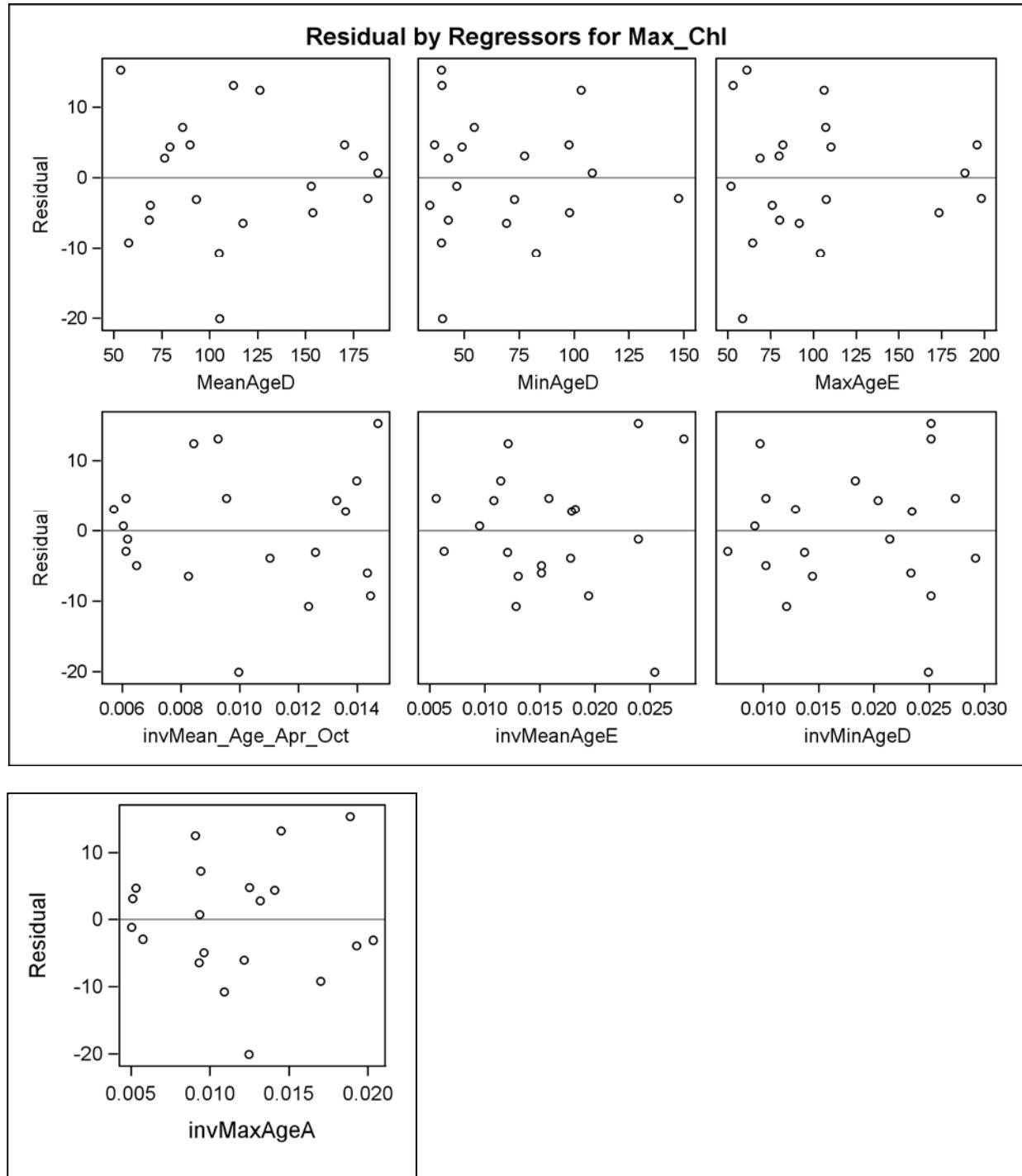
Appendix 8.C.



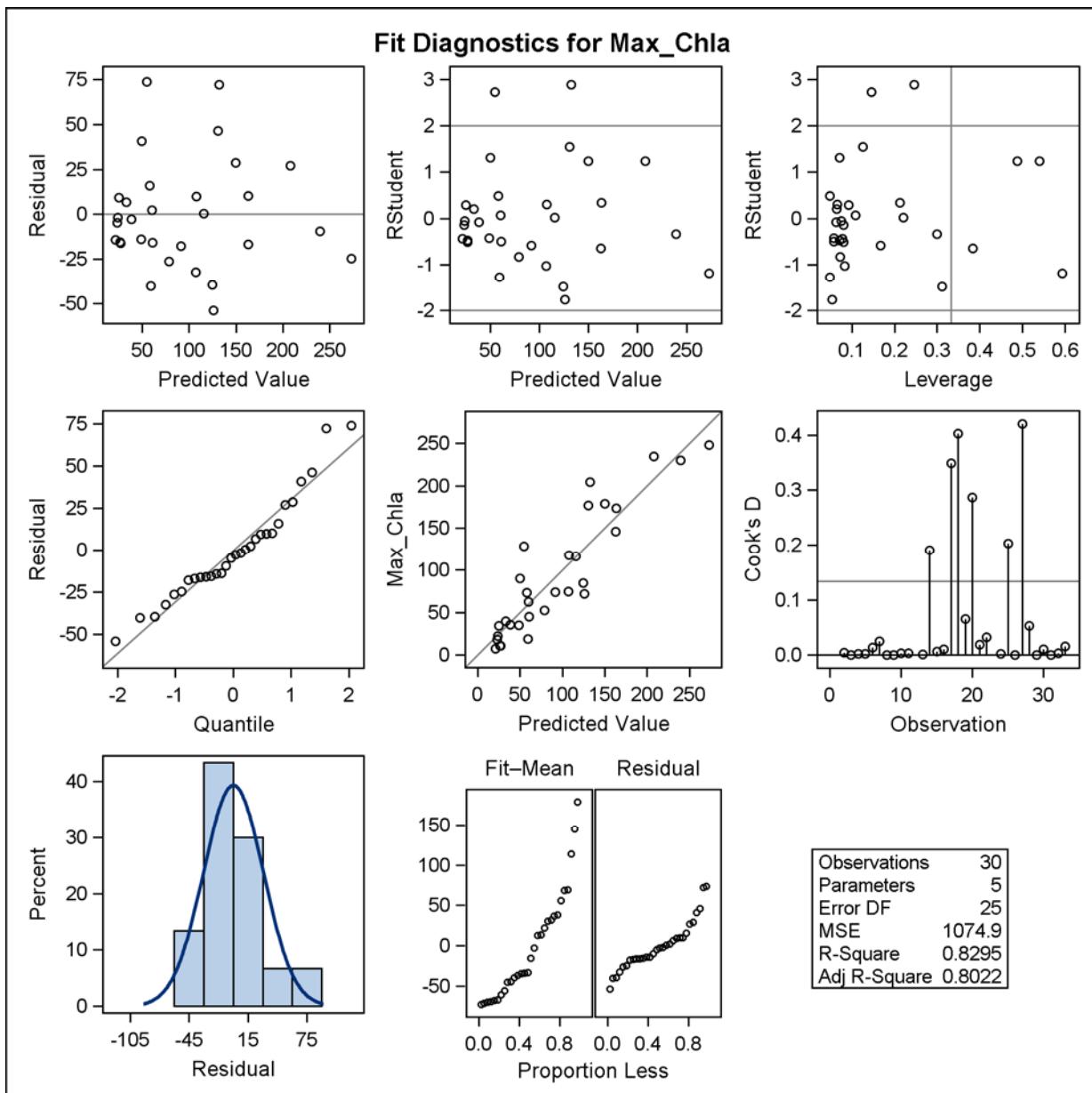
M. Freshwater Maximum Chl-a, Segments 3 & 4



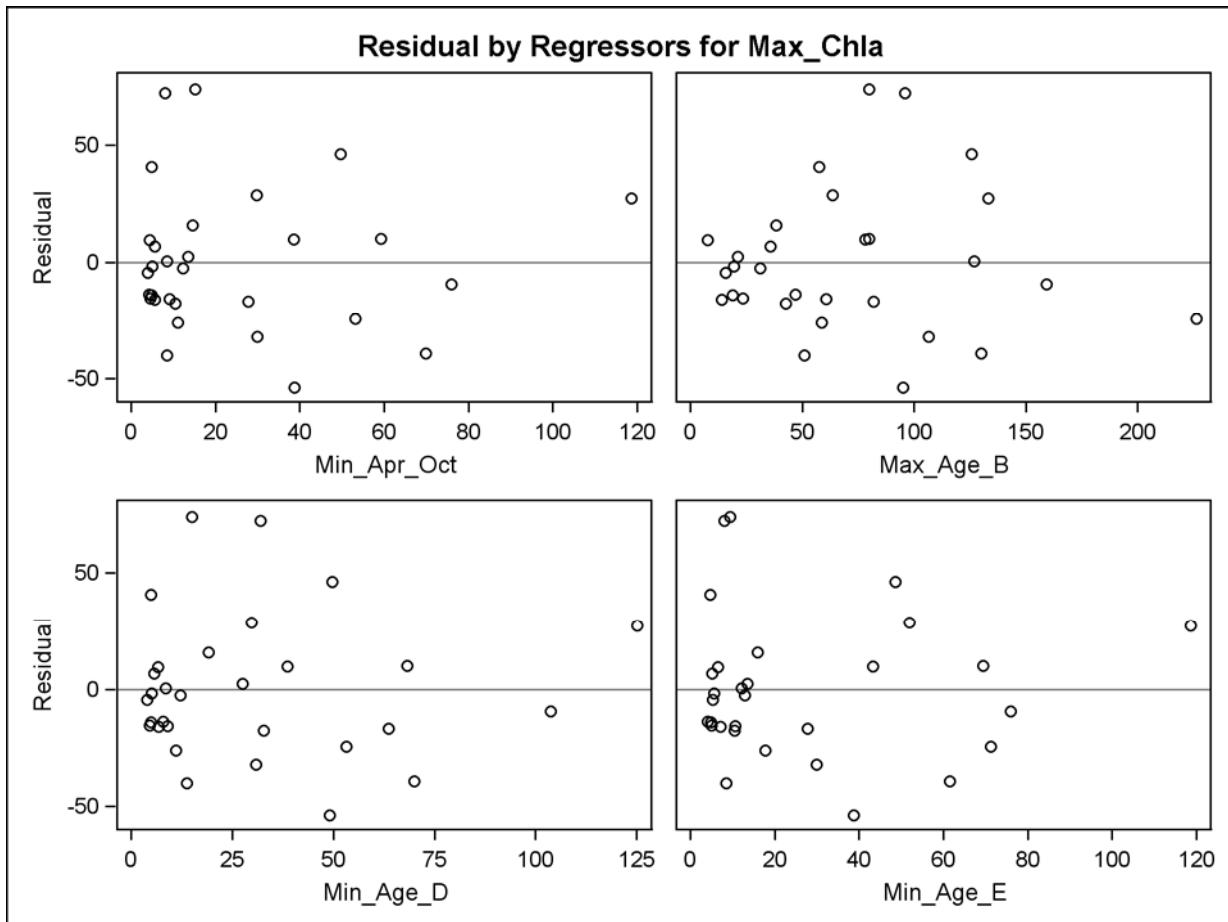
Appendix 8.C.



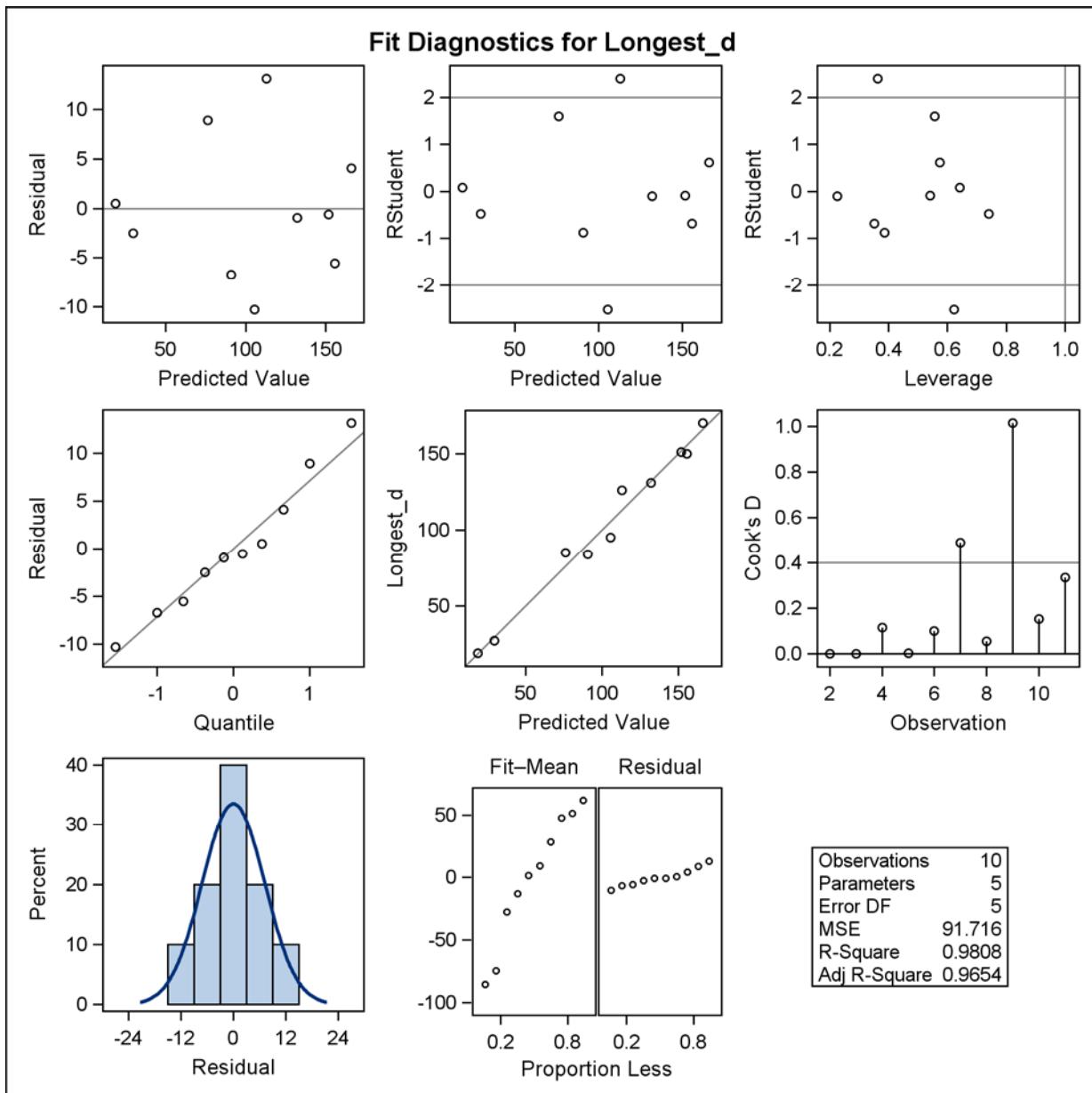
N. Freshwater Maximum Chl-a, Segment 6



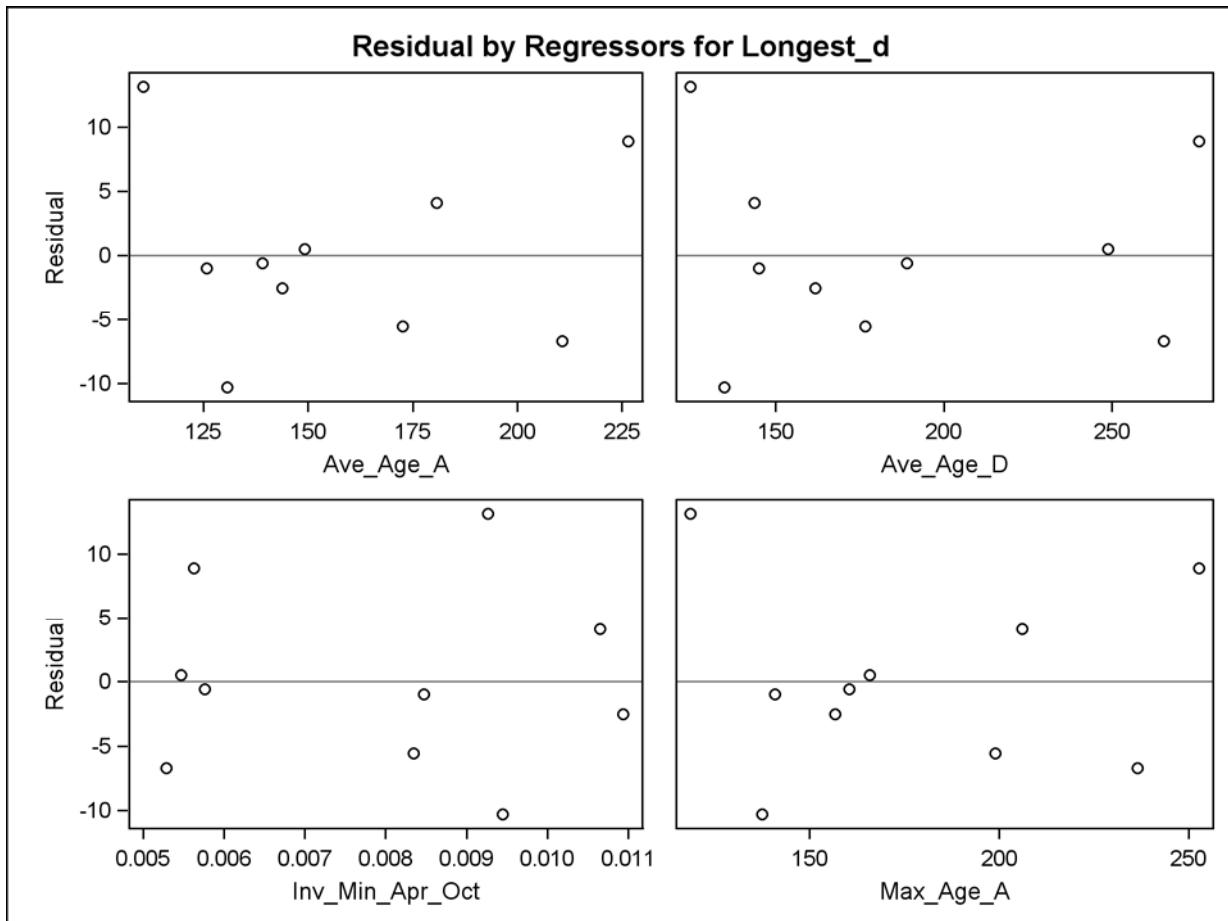
Appendix 8.C.



O. Freshwater Bloom Duration, Segment 2

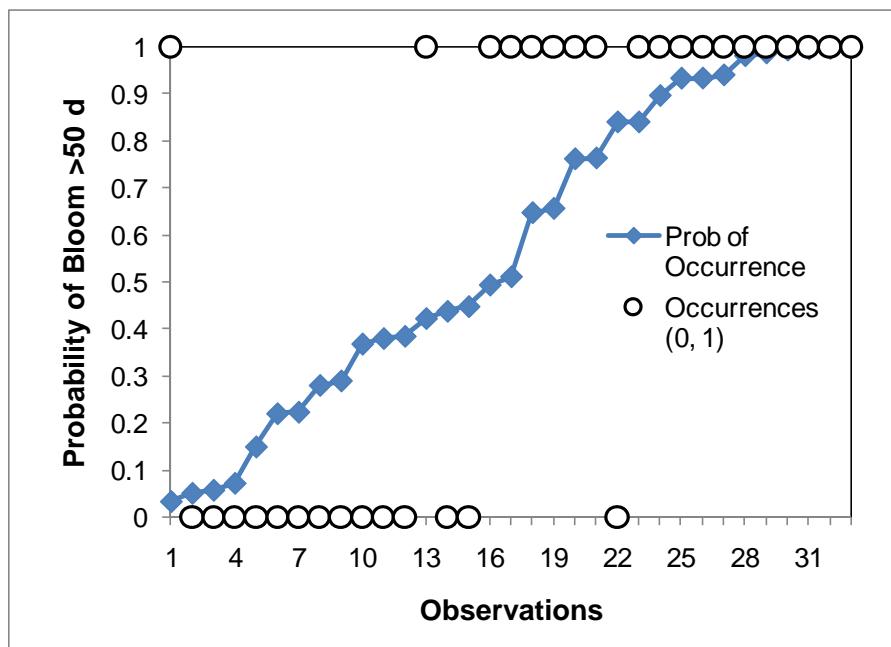


Appendix 8.C.

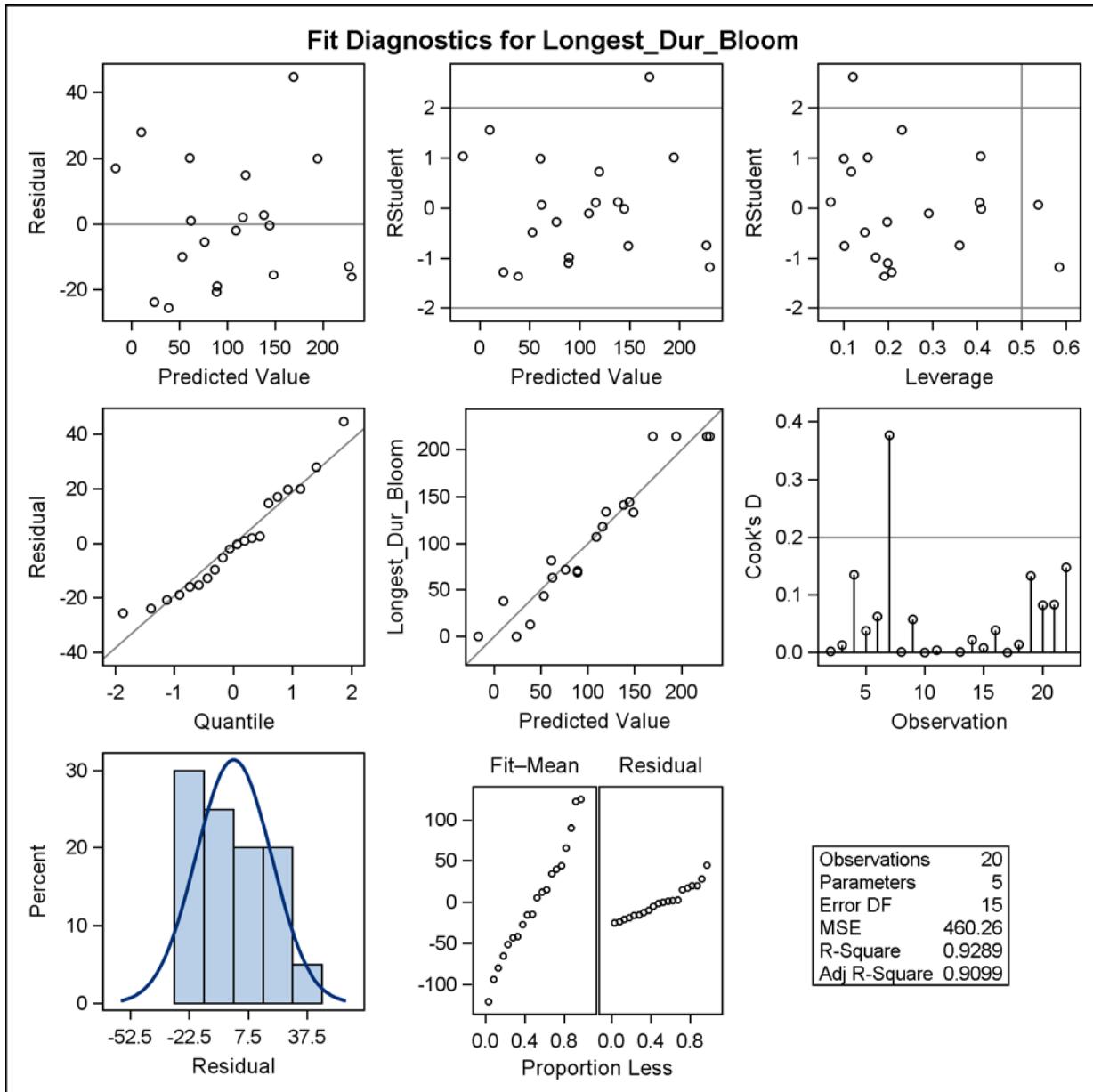


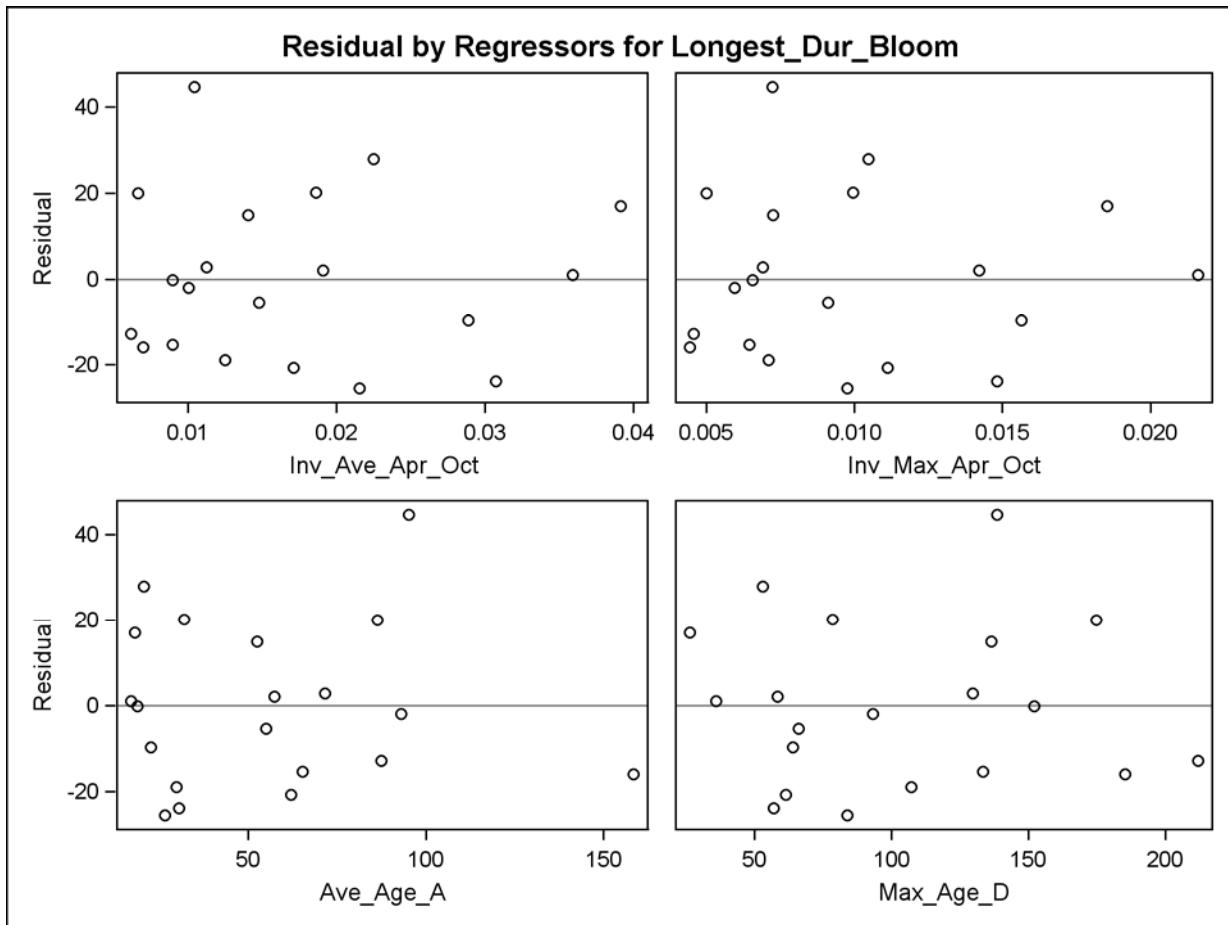
P. Freshwater Bloom Duration, Segments 3 & 4

This regression model used logistic rather than linear regression, and goodness-of-fit metrics are included in model calculation (above) rather than summarized in graphics. The figure below shows observations (coded 1 = occurrence of bloom >50 d, or 0 = no occurrence) versus the probability of a bloom >50 d predicted by the binomial logistic regression. The overall regression was significant (likelihood ratio test of global null hypothesis, $p < 0.001$), and both regression coefficients were significant (Wald maximum likelihood chi-square, $p < 0.05$). The Hosmer-Lemeshow goodness-of-fit test confirmed that the observed frequency of events did not differ significantly from that predicted by the regression (chi-square, $p > 0.05$) (see model calculation results above).



Q. Freshwater Bloom Duration, Segment 6





References

SAS Institute Inc. 2010. SAS/STAT® 9.22 User's Guide. Cary, NC: SAS Institute Inc.