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**Appendix C** 

## Application of a General Linear Model (GLM) to the Analysis of CVOC Historical Case Data

# Appendix C

### Application of a General Linear Model (GLM) and an Analysis of Covariance (ANCOVA)

### C.1. Background

As stated in Appendix A, it is presumed that plume length will co-vary with other important variables, such as the strength of the source term or groundwater velocity, in addition to reductive dehalogenation. In this case, the form of the general linear model corresponds to an analysis of covariance or ANCOVA (Steel and Torrie, 1980), where the variable referred to as "EVIDENCE" is considered the treatment effect in the presence of other modeled covariates. Note, incidentally, that this statistical analysis is based on observational and not experimental data. Plumes were not randomly assigned to the treatment conditions.

It is important to define the scope of inference regarding the conclusions of these statistical analyses. To reliably generalize the interpretation of these results to the entire population of CVOC plumes in the United States, a randomly selected sample of *N* plumes from the identified or target population would have to be sampled. This was certainly not the case in this study. In fact, defining this **population may be a cost-prohibitive exercise**. **Instead, the more practical strategy has been to identify** and obtain data on CVOC plumes from a broad geographic area with the intent to secure a representative sample. The conclusions under the theoretical scope of inference can be made with confidence and quantifiable uncertainty, but practicality necessitates settling for reasonable reliability instead.

### C.2. General Linear Model Description and Results

In order to perform analysis of covariance (ANCOVA) by a general linear model for log plume length, three indicator or dummy variables were first created:

 $ind1 = \begin{cases} 1, if EVIDENCE is "STRONG" \\ 0, otherwise \\ ind2 = \\ 1, if EVIDENCE is "WEAK" \\ 0, otherwise \\ 1, if EVIDENCE is "NONE" \\ 0, otherwise \end{cases}$ 

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In addition, the two covariates (log(max.conc.) and log(meanV, where V is groundwater velocity) were multiplied by each of the indicator variables which produced the following new variables defined as:

$$XC_{1} = \frac{log(max.conc.), \text{ if EVIDENCE is "STRONG"}}{0, \text{ otherwise}}$$
$$XC_{2} = \frac{log(max.conc.), \text{ if EVIDENCE is "WEAK"}}{0, \text{ otherwise}}$$
$$XC_{3} = \frac{log(max.conc.), \text{ if EVIDENCE is "NONE"}}{0, \text{ otherwise}}$$

and,

$$XV_{1} = \frac{log(meanV), \text{ if EVIDENCE is "STRONG"}}{0, \text{ otherwise}}$$
$$XV_{2} = \frac{log(meanV), \text{ if EVIDENCE is "WEAK"}}{0, \text{ otherwise}}$$
$$XV_{3} = \frac{log(meanV), \text{ if EVIDENCE is "NONE"}}{0, \text{ otherwise}}$$

Therefore, this system of coding for the general linear model, allows us to fit a "full model"

$$Y_{i} = \beta_{01} ind_{1i} + \beta_{02} ind_{2i} + \beta_{03} ind_{3i} + \beta_{11} XC_{1i} + \beta_{12} XC_{2i} + \beta_{13} XC_{3i} + \beta_{21} XV_{1i} + \beta_{22} XV_{2i} + \beta_{23} XV_{3i} + \varepsilon_{i}$$
(Eq. C-1)

and a "reduced model"

$$\mathbf{Y}_{i} = \beta_{01} \operatorname{ind}_{1i} + \beta_{02} \operatorname{ind}_{2i} + \beta_{03} \operatorname{ind}_{3i} + \beta_{1} \log(\max \operatorname{conc.}) + \beta_{2} \log(\operatorname{meanV}) + \varepsilon_{i} \qquad (\text{Eq. C-2})$$

The full model (Eqn. C-1) allows the bivariate linear regressions of the log of plume length (Y) on the log of maximum concentration and the log of mean groundwater velocity to be fit separately for each level of the main effect, EVIDENCE. For example,  $Y_{ji}$ , the i<sup>th</sup> measurement of log plume length for plumes where j = 1 representing STRONG evidence of reductive dehalogenation, can be described by the sub-model:

$$Y_{1i} = \beta_{01} ind_{1i} + \beta_{11} X C_{1i} + \beta_{11} X V_{1i} + \varepsilon_i$$
 (Eq. C-3)

Similar sub-models can be identified for each of the other two levels of EVIDENCE (i.e., WEAK and NONE). This means that the slope parameters of the regression relationships described above for each level of EVIDENCE are free to vary, viz., they are heterogeneous.

This model is tantamount to a completely specified model for an ANCOVA. The advantage of fitting Eqn. C-1 is that all parameters among all levels of EVIDENCE can be fit simultaneously.

By the method known as reduction sum of squares (Searle 1987), we can test the hypothesis that any  $Y_{ji}$  can be described simply as a function of the intercept parameter ( $_{0j}$ ) for the j<sup>th</sup> level of EVIDENCE and common slope parameter for each covariate ( $_{1j}$ ,  $_{2j}$ ). This hypothesis assumes that the slope parameters among the covariates are homogeneous, ( $_{k1} = _{k2} = _{k3}$ , k=1,2), for the k<sup>th</sup> covariate.

We then calculate the statistic:

$$F = \frac{(SSE_{reduced model} - SSE_{full model})}{MSE_{full model}}$$
no. of parameters  
(Eq. C-4)

where SSE is the error sum of squares for each of the two models.

The statistic in Eq. C-4 is distributed as a  $F_{n1,n2}$  distribution with numerator degrees of freedom (n1) equal to difference ( ) in the number of parameters specified in the full and reduced models, and the denominator degrees of freedom (n2) equal to that corresponding to the mean squared error (MSE) of the full model.

From the analysis results given in Tables C-1a through C-1e and C-2a through C-2e, performed using the JMP (version 3.2.1) software from SAS Institute,

$$F_{4,120} = \frac{(26.540697 - 26.031044)/4}{.216925} = 0.587$$

If the homogeneous slopes hypothesis is true, we would expect to obtain an F statistic as large or larger than 0.587 approximately 70% of the time (i.e., p = 0.672). We may conclude that there is insufficient evidence for rejecting this hypothesis with a power for detecting slope heterogeneity, if there was any, about 98% of the time.

Furthermore, a test for whether or not plumes with STRONG evidence of reductive dehalogenation are shorter than plumes with either WEAK or no (NONE) evidence is a matter of comparing the intercept parameters ( $_{0j}$ ) in the reduced model. Specifically, we can test whether or not  $_{01}$ - $_{0j}$ <0 [for j=2(WEAK), 3(NONE)]; this can be accomplished by performing a standard ANCOVA, again using the JMP software, with corresponding paired comparisons among the least squares means presented in Tables C-3a through C-3h, Tables C-4a through C-4h, and Plots C-3c through C-4f.

### C.3. ANCOVA Results

A plot of the CVOC plume length means on the log scale for all CVOCs with six or more recorded plumes is shown on Figure C-1. In order to justify the use of the entire data set in the subsequent statistical model, it is important to demonstrate that there are no statistically significant differences in plume length among the several CVOC species. The overall mean plume length is shown on Figure C-1 as the horizontal line crossing the entire plot. The center line within each diamond indicates the mean plume length for that CVOC species the top and

bottom of the diamond indicates the upper and lower 95% confidence limits, respectively, using a pooled estimate of plume length variance among all plumes. The diameter of the comparison circles to the right of the means plot is proportional to the standard deviation of plume lengths on the log scale. The angle formed by two tangent lines between overlapping circles is an indication of the statistical significance of that comparison. If the angle formed is  $< 90^{\circ}$  then we may conclude that the given pair of CVOCs is statistically different with a 5% chance or less of error (p < 0.05). These circles suggest little evidence for a practical difference in plume length among CVOCs. An analysis of variance (ANOVA) (Steel and Torrie, 1980) test also indicates that there is indeed insufficient evidence for a statistically significant difference among CVOC plume lengths (p = 0.14) at the 5% level (i.e., the error rate for false positive conclusions).

One other important assumption prior to conducting an ANCOVA is to test the assumption that the log of plume lengths is normally distributed. A histogram of these plume lengths on the log scale, a box-and-whisker plot, and a normal quantile plot are all shown on Figure C-2. Each plot is designed to show the strength of the evidence for the normality assumption. A theoretical normal (bell) curve is superimposed on the histogram whose mean is the sample mean of the plume length logarithms. The box-and-whisker plot shows the quantiles where the horizontal bar is the median (50th percentile) and the top and bottom of the box are the 75th and 25th percentiles, respectively. The diamond indicates the mean, which, if the sample data are normally distributed, should be nearly identical to the median. The normal quantile plot shows the theoretical quantile of the data as standard normal deviates on the abscissa and the actual values (logs) of plume lengths on the ordinate axis. If the data derive from a normal distribution, the data would all fall along a straight line. This plot indicates that the shortest plume lengths are shorter than expected under the lognormal probability distribution model. Furthermore, an inference test of normality (Shapiro-Wilk *W*-Test) indicates a statistically significant departure from this assumption (p = 0.0004).

Given the results of the normality test, an additional ANCOVA was performed on the ranks of the plume length as an equivalent non-parametric test (Conover, 1980). This test again indicated no significant difference in plume lengths among CVOC species (p = 0.40).

The relationship between the plume length and each of the two covariates, maximum concentration and mean velocity, respectively, are shown on the log scale on Figures C-3 and C-4. Three difference linear regression lines are also shown in each plot, one for a separate fit for each category of EVIDENCE. With the exception of plumes showing strong evidence of reduction dehalogenation in Figure C-4, the slopes of these relationships are very similar. The aim of the subsequent GLM was to test, simultaneously, whether these slopes are can be considered equal to one another by a comparative reduction in the error sum of squares between two models, one which assumes equal slopes and one which does not (Searle, 1987). If so, the ANCOVA test for differences in mean plume lengths between evidence categories is tantamount to comparing the intercepts in Figures C-3 and C-4. The results of this analysis are provided in the Appendix A. The GLM results indicated insufficient evidence for concluding that these slopes are different (p = 0.672). The resulting and simplified ANCOVA model justifiably contains only a main effect term for EVIDENCE and the two covariates with a common slope parameter for each covariate. The ANCOVA results indicated a significant and positive relationship between plume length and only two covariates, maximum concentration (p < 0.001) and mean velocity (p = 0.008). In this analysis, there were 129 of the 243 plumes described earlier for which complete data for EVIDENCE and covariates were measured.

The least squares mean plume lengths for each category of EVIDENCE on the original and log scale resulting from the ANCOVA are presented on Table C-2. Least squares mean plume lengths are sample means adjusted for the relationships with the covariates. As indicated on the table, plumes with strong evidence of reductive dehalogenation are shorter than plume lengths with either weak or no evidence. The ANCOVA results indicate that these two paired comparisons of plume length means are statistically significant, p = 0.004 and p = 0.003, respectively.

An ANCOVA was also performed on the ranks of plume lengths as a corresponding equilvalent nonparametric test. The conclusions were similar, viz., that a significant and positive relationship exists between plume length and only two covariates, maximum concentration (p < 0.0001) and mean velocity (p = 0.0014), and that the mean plume lengths are significantly shorter when there is strong evidence of reductive dehalogenation as compared to plumes with weak (p = 0.001) or no evidence (p = 0.002).

A plot of the cumulative distribution of the residuals from the ANCOVA model displayed separately for each category or level of EVIDENCE, in order from smallest to largest, is presented on Figure C-5. A residual is the difference between the fitted value from the model and the actual value. Residuals are normally distributed with a mean equal to zero. This means that there are positive residuals (i.e., plumes longer than expected by the model) and negative residuals (i.e., plumes shorter than expected by the model). Consequently, accumulating the values of residuals, from smallest to largest, will yield an inverted parabola shape to the cumulative distribution function. If there were no difference between the levels of EVIDENCE, these inverted parabolas would overlay each other. Instead, not only are they separated but there are different minimum values for each.

The smallest minimum value in Figure C-5, occurs among residuals for those plumes with the strongest evidence of reductive dehalogenation. This indicates that there were shorter plumes (i.e., more negative residuals) in this level of EVIDENCE than in any other. The maximum for each cumulative distribution in Figure C-5, is zero because the sum of the residuals is zero. These maximums occur at a different value of order corresponding to the samples size or number of plumes in each level of EVIDENCE.

As in the previous data analysis by cumulative distribution of plume length indices (see Appendix A), the cumulative distribution of residuals from an ANCOVA model corroborates the finding that the shortest CVOC plumes are associated with the strongest evidence of reductive dehalogenation.

An additional ANCOVA was performed on a subset of the CVOC data that excluded "daughter" plumes. Such plumes are derived from the breakdown of other CVOC species and were used to define the EVIDENCE category. This analysis is an attempt to eliminate a suspected data bias or over representation of shorter plumes in the larger data set. Therefore, data from sixteen cis-1,2-DCE, and seven vinyl chloride plumes were deleted from the previous data set containing 129 plumes with complete information for all variables in the statistical model. A second ANCOVA was then performed.

The analysis of the subsequent 106 CVOC plumes showed that both maximum concentration and mean velocity were still statistically important (p = 0.002 and p = 0.083, respectively) in explaining the variation in the log of plume length. However, mean velocity was substantially less helpful than maximum concentration, contrary to the earlier ANCOVA results which used all of the CVOC plumes (see Tables C-3 and C-4). But having accounted for the variation in log plume length due to these two covariates, we may still conclude with confidence that plumes exhibiting strong EVIDENCE of reductive dehalogenation are significantly shorter than plumes with either weak or no EVIDENCE (p = 0.003 and p = 0.004, respectively).

Table C-5 shows that the statistical bias-corrected (Gilbert 1987) estimates of the median plume length (with or without the daughter plumes), when there is strong EVIDENCE of reductive dehalogenation, is about half as long as a plume showing either weak or no EVIDENCE.

### References

Conover, W. J (1980), Practical Nonparametric Statistics (2nd ed.), Wiley, New York.

Gilbert, R. O. (1987), Statistical Methods for Environmental Pollution Monitoring, Van Nostrand Reinhold Co., New York.

Searle, S. R. (1987), Linear Models for Unbalanced Data (Wiley, New York).

Steel, R. G. D., and Torrie, J. H. (1980), Principles and Procedures of Statistics: A Biometrical Approach (2<sup>nd</sup> Edition), McGraw-Hill Book Co., New York.

### Tables C-1.

Table C-1a. Response: Log (Length) Summary of Fit.

Statistical parameters	Statistical results
R Square	0.197504
R Square (adjusted)	0.144004
Root Mean Square Error	0.465752
Mean of Response	2.929986
Observations (or sum of weights)	129

#### Table C-1b. Parameter estimates.

Term	Estimate	Std error	t ratio	<b>Prob</b> > [t]
Intercept	Zeroed	0	0	-
ind1	2.0703486	0.273666	7.57	<0.0001
ind2	2.8842836	0.245101	11.77	<0.0001
ind3	2.593284	0.211894	12.24	<0.0001
XC1	0.1252731	0.075691	1.66	0.1005
XC2	0.0964387	0.062325	1.55	0.1244
XC3	0.170673	0.065222	2.62	0.0100
XV1	0.5525953	0.242685	2.28	0.0246
XV2	-0.12301	0.076677	-1.60	0.1113
XV3	-0.106314	0.091102	-1.17	0.2455

Table C-1c. Effect test.

Source	Nparm	DF	Sum of squares	F ratio	<b>Prob</b> > <b>F</b>
ind1	1	1	12.415234	57.2327	<0.0001
ind2	1	1	30.039765	138.4797	<0.0001
ind3	1	1	32.491845	149.7835	<0.0001
XC1	1	1	0.594207	2.7392	0.1005
XC2	1	1	0.519386	2.3943	0.1244
XC3	1	1	1.485411	6.8476	0.0100
XV1	1	1	1.124702	5.1847	0.0246
XV2	1	1	0.558285	2.5736	0.1113
XV3	1	1	0.295418	1.3618	0.2455

Source	DF	Sum of squares	Mean square	F ratio
Model	8	6.406547	0.800818	3.6917
Error	120	26.031044	0.216925	Prob > F
C Total	128	32.437591	_	0.0007

Table C-1d. Whole model test - Analysis of variance
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Tested against reduced model: Y = mean.

### Table C-1e. Whole model test – Power.

Alpha	Sigma	Delta	Number	Power
0.0500	0.465752	0.222852	129	0.9821

### **Tables C-2**

Table C-2a. Response: Log(length) summary of fit.

Statistical parameters	Statistical results
R Square	0.181792
R Square (adjusted)	0.155398
Root Mean Square Error	0.462642
Mean of Response	2.929986
Observations (or sum of weights)	129

### Table C-2b. Parameter estimates.

Term	Estimate	Std error	t ratio	<b>Prob</b> > [t]
Intercept	Zeroed	0	0	-
ind1	2.3384006	0.141013	16.58	<0.0001
ind2	2.6579117	0.139423	19.06	<0.0001
ind3	2.6539975	0.130973	20.26	<0.0001
log(Max. conc.)	0.1432315	0.038348	3.74	0.0003
log(Mean V)	0.1039279	0.038225	2.72	0.0075

Max. conc. = maximum concentration.

#### Table C-2c. Effect test.

Source	Nparm	DF	Sum of squares	F ratio	Prob > F
ind1	1	1	58.859002	274.9934	<0.0001
ind2	1	1	77.785787	363.4207	<0.0001
ind3	1	1	87.887664	410.6173	<0.0001
log(Max. conc.)	1	1	2.985910	13.9504	0.0003
log(Mean V)	1	1	1.582174	7.3920	0.0075

Max. conc. = maximum concentration.

Source	DF	Sum of squares	Mean square	F ratio
Model	4	5.896894	1.47422	6.8877
Error	124	26.540697	0.21404	Prob > F
C Total	128	32.437591	_	<0.0001

Tested against reduced model: Y = mean.

### Table C-2e. Whole model test – Power.

Alpha	Sigma	Delta	Number	Power
0.0500	0.462642	0.213804	129	0.9928

### Tables and Plots C-3 ANCOVA Results - All CVOC Plumes

Table C-3a. Response: Log(length) summary of fit.

Statistical parameters	Statistical results
R Square	0.181792
R Square (adjusted)	0.155398
Root Mean Square Error	0.462642
Mean of Response	2.929986
Observations (or Sum of weights)	129

#### Table C-3b. Effect test.

Source	Nparm	DF	Sum of squares	F ratio	Prob > F
log (Max. conc.)	1	1	2.9859101	13.9504	0.0003
log (Mean V)	1	1	1.5821737	7.3920	0.0075
Evidence	2	2	2.4974348	5.8341	0.0038

Max. conc. = maximum concentration.



#### Plot C-3c. Whole Model Test

Table C-3c. Whole model test - Analysis of variance.

Source	DF	Sum of squares	Mean square	F ratio
Model	4	5.896894	1.47422	6.8877
Error	124	26.540697	0.21404	Prob > F
C Total	128	32.437591	-	<.0001





Table C-3d. Effect test - Log (max. conc.).

Sum of squares	F ratio	DF	<b>Prob</b> > <b>F</b>
2.9859101	13.9504	1	0.0003



Table C-3e. Effect test - Log (mean V).

Sum of squares	F ratio	DF	Prob > F
1.5821737	7.3920	1	0.0075





Table C-3f. Effect test – Evidence.

Sum of squares	F ratio	DF	<b>Prob</b> > <b>F</b>
2.4974348	5.8341	2	0.0038

Level	Least sq mean	Std error	Mean
NONE	3.018958411	0.0726928309	2.98939
STRONG	2.703361502	0.0778543976	2.75946
WEAK	3.022872630	0.0659426758	3.00595

### Table C-3g. Least squares means – Evidence.

### Table C-3h. Contrast – Evidence.

Variables	Result	Result
NONE	-1	0
STRONG	1	1
WEAK	0	-1
Estimate	-0.316	-0.32
Std Error	0.1068	0.1037
t Ratio	-2.955	-3.08
Prob> t	0.0037	0.0026
SS	1.8691	2.0303

Statistical parameters	Statistical results
Sum of Squares	2.4974347715
Numerator DF	2
F Ratio	5.8340953965
Prob > F	0.0037888412

### Tables and Plots C-4 ANCOVA Results: Without CVOC daughter plumes

#### Table C-4a. Response: Log(length) summary of fit.

Statistical parameters	Statistical results
R Square	0.175685
R Square (adjusted)	0.143039
Root Mean Square Error	0.449819
Mean of Response	2.944213
Observations (or Sum of weights)	106

#### Table C-4b. Effect test.

Source	Nparm	DF	Sum of squares	F ratio	<b>Prob</b> > <b>F</b>
log(max. conc.)	1	1	2.0757387	10.2588	0.0018
log(mean V)	1	1	0.6184906	3.0567	0.0834
Evidence	2	2	2.2501787	5.5605	0.0051

Max. conc. = maximum concentration.



Plot C-4c. Whole Model Test

Table C-4c. Whole model test - Analysis of variance.

Source	DF	Sum of squares	Mean square	F ratio
Model	4	4.355518	1.08888	5.3815
Error	101	20.436047	0.20234	Prob > F
C Total	105	24.791565	-	0.0006





Table C-4d.	Effect test	- Log(maximum	concentration).
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Sum of squares	F ratio	DF	Prob > F
2.0757387	10.2588	1	0.0018



Table C-4e. Effect test – Log (mean V).

Sum of squares	F ratio	DF	<b>Prob</b> > <b>F</b>
0.61849063	3.0567	1	0.0834



Table C-4f. E	ffect test -	<b>Evidence</b> .
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Sum of squares	F ratio	DF	<b>Prob</b> > <b>F</b>
2.2501787	5.5605	2	0.0051

Level	Least sq mean	Std error	Mean
NONE	3.016290076	0.0708913245	2.98939
STRONG	2.680907406	0.0903285548	2.72666
WEAK	3.043977628	0.0738156225	3.04176

### Table C-4g. Least Squares Means – Evidence.

### Table C-4h. Contrast – Evidence.

Variables	Result	Result
NONE	-1	0
STRONG	1	1
WEAK	0	-1
Estimate	-0.335	-0.363
Std Error	0.1149	0.1187
t Ratio	-2.92	-3.058
Prob> t	0.0043	0.0029
SS	1.7249	1.8916

Statistical parameters	Statistical results
Sum of Squares	2.2501786762
Numerator DF	2
F Ratio	5.5604698798
Prob > F	0.0051174022

Evidence <sup>a</sup>	Sample size <sup>b</sup>	Mean <sup>c</sup>	Least squares mean <sup>c</sup>	Standard error <sup>c</sup>	Geometric mean <sup>d</sup> (original scale)
Data: All CVOC plumes					
Strong	37	2.759	2.703	0.078	508.2
Weak	51	3.006	3.023	0.066	1.059.7
None	41	2.989	3.019	0.073	1,051.2
Data: Without CVOC Daughter Plumes					
Strong	26	2.727	2.681	0.090	484.2
Weak	39	3.042	3.044	0.074	1,113.6
None	41	2.989	3.016	0.071	1,043.6

# Table C-5. Plume length means, least squares means and statistics from an analysis of covariance (ANCOVA) - log and original scale (ft).

<sup>a</sup> Evidence of reductive dehalogenation.

<sup>b</sup> Number of plumes in each category of Evidence.

<sup>c</sup> Rounded to three decimal places.

<sup>d</sup> The bias corrected (Gilbert 1987) geometric mean is a sample estimate of the median (i.e., 50<sup>th</sup> percentile) on the original scale.



Figure C-1. Plot of CVOC means and ANOVA test results.



Figure C-2. Normality assumption test statistics for the common logs of plume length by histogram, box-and-whisker plot, normal quantile plot, and inference test results.



Figure C-3. Plot of Log (length) vs Log (max. conc.) for each category of evidence for reductive halogenation.



Figure C-4. Plot of Log (length) vs Log (mean V) for each category of evidence for reductive halogenation.



Figure C-5. Cumulative distributions of residuals from the ANCOVA model. The small minimum value for the strong reductive dehalogenation set is indicative of shorter-than-expected plume lengths after taking source concentration and groundwater velocity covariates into account. See text for explanation.