Prepared for:

SETTLING DEFENDANTS

Revision 1

CO-LOCATION OF DIOXINS/FURANS AND AROCLOR 1268

LCP CHEMICALS SITE OPERABLE UNIT 1 BRUNSWICK, GEORGIA

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February 2019

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Senior Principal

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1 INTRODUCTION

1.1 Background and Executive Summary

This co-location study was performed in accordance with Appendix B of the Consent Decree between Honeywell and the Georgia Power Company ("GPC") with the United States Environmental Protection Agency ("USEPA"), *The United States v. Honeywell International Inc. et al.*, Civil Action No. 2:16-cv-00112, which was filed in the United States District Court for the Southern District of Georgia, with an effective date of July 27, 2017 ("Consent Decree"). Collectively, Honeywell and GPC are herein referred to as the Settling Defendants ("SDs"). The Consent Decree addresses the salt marsh that constitutes Operable Unit 1 ("OU1") of the LCP Chemicals Superfund Site in Brunswick, Georgia ("Site").

USEPA examined past sampling for PCDD/Fs at the Site and local area in a memorandum as part of the Record of Decision ("ROD") for OU1 (USEPA, 2014, 2015). The memorandum provided an evaluation on the association (*i.e.*, co-location) of polychlorinated dibenzodioxins/furans ("PCDD/F") in OU1 sediments with Aroclor 1268, presenting evidence that a high degree of co-location exists. Due to the somewhat limited PCDD/F data set used in the 2014 evaluation, USEPA concluded in the memorandum that "additional [PCDD/F] sampling will be required to confirm the dioxin furans conceptual site model, *i.e.*, that Aroclor 1268 and dioxin furans are co-located and that remediating the former will reduce dioxin furans concentrations to acceptable levels."

The present study conducted in 2018 involved strategic sampling targeting the various portions of OU1 designated for Remedial Action, contributing numerous additional characterization points in OU1 to supplement prior OU1 sampling for paired Aroclor 1268 and PCDD/F testing. In doing so and based on the collaborating results of the 2018 co-location study, the Conceptual Site Model ("CSM") developed in 2014 by the USEPA is further validated.

The statistical evaluation provides clear and meaningful evidence of the strong association of PCDD/F with Aroclor 1268 in the OU1 sediments. This allows the following factors to support the conclusions developed from the Aroclor 1268 characterization in OU1, to be applied to PCDD/F, and no further assessment is necessary. In summary:

1. The paired test results support the CSM regarding co-location, and thus remediating the PCB condition will remediate a similar PCDD/F condition.
2. The highest PCDD/F condition occurs in the portion of Eastern Creek beyond the area of the past Removal Action dredging, where the highest condition in Eastern Creek should be expected (according to the CSM).

It is well documented that the tidal channel sediments exhibit a significantly higher contaminant condition relative to the adjoining marsh flats. Remediating the full extent of Eastern Creek in the OU1 Remedial Action will address the elevated dioxin toxic equivalency ("TEQ") present in that channel.

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1.2 Terms of Reference

According to 3.1(f)(1) of Appendix B (Statement of Work) of the Consent Decree: "[The Pre-Design Study (PDS)] includes verification sampling to confirm that polychlorinated dibenzodioxins/polychlorinated dibenzofurans ("PCDD/Fs") and Aroclor 1268 are co-located." (USEPA, 2016). The study design was provided in the *Co-location Study Work Plan* (Appendix B to the *Remedial Design Work Plan*) dated March 28, 2018 and approved by the USEPA on April 16, 2018.

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2 CONCEPTUAL SITE MODEL – ASSOCIATION OF PCDD/F WITH AROCLOR 1268

2.1 Site Setting

The Site occupies approximately 880 acres immediately northwest of the City of Brunswick, Glynn County, Georgia (Figure 1) and is comprised of approximately 760 acres of salt marsh and 120 acres of high ground (uplands). The upland area, where manufacturing operations at the Site occurred, is bordered by the Glynn County Detention Center and Public Works to the north, Ross Road to the east, and Brunswick Cellulose to the south.

2.2 OU1 Features

The LCP marsh is characterized by vegetated marsh flats dissected by numerous channels and larger creeks under tidal influence from Turtle River. These features provide a physical segregation of OU1 into "domains", as illustrated on Figure 2. The principal feature of the marsh is Purvis Creek, which enters the marsh on the Site from the Turtle River at the southwest corner and ends at the northeast upland-marsh border. Smaller tidal channels and creeks existing in the LCP marsh include the Main Canal, Eastern Creek, Western Creek Complex, Landfill Creek, and Domain 3 Creek (Figure 2).

2.3 Release of Aroclor 1268 and PCDD/F Compounds to OU1

From 1913 to the mid-1970s, chlor-alkali processes commonly used graphite blocks as anodes in the electrolysis process (O'Brien *et al.*, 2005). The graphite anodes contained coal tar pitch as a bonding agent, and cyclic aromatic compounds (such as dibenzofuran) were common constituents of the coal tar pitch. Successive chlorination of cyclic aromatic compounds present in the coal tar has been proposed as the primary mechanism for formation of PCDFs during the chlor-alkali process (consistent with the findings of Yamamoto *et al.*, 2017).

Graphite block anodes were used at the Site until the mid-1970s. Furthermore, Aroclor 1268 which is a form of polychlorinated biphenyls ("PCBs"), was impregnated into the graphite anodes for a period of time in the 1960s to condition the anode block prior to placement in the electrolytic cell. Thus, Aroclor 1268 was also characteristic of the graphite sludge at the Site.

The facility also generated process wastewater, which prior to the enactment of the Clean Water Act in 1972, was discharged with little treatment to the marsh (Domain 1). During the ebb tide cycle, these waters would follow the Main Canal to Purvis Creek. During the flood tide cycle, water flow reversed "upstream" serving to push the diluted wastewater stream into Eastern Creek

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and into the upper reaches of Purvis Creek (Figure 3). At the approximate middle portion of the flood tide, the water level overtops the banks of the tidal channels flooding the marsh flats, spreading to the point of the "tidal node" where it meets flood tide waters from an adjacent channel. During high tide, suspended contaminated particles could be transported over the banks into the marsh. However, once out of the channel, the rapid increase in cross-sectional area and resistance to flow caused by the marsh grasses lowers water velocities and limits the transport distance of particulate-bound chemicals into the marsh (ENVIRON and Anchor QEA, 2013).

2.4 Physical-Chemical Properties

PCBs such as Aroclor 1268, and PCDD/Fs are nonpolar compounds and are characterized as hydrophobic. With a log $K_{OW} > 7.4$, Aroclor 1268 partitions strongly to non-polar substances (*e.g*, organic matter). PCDD/Fs exhibit similar behavior (tetrachlorinated PCDD compounds have a log $K_{OW} > 6.8$). Because of the strong hydrophobic composition of Aroclor 1268 and PCDD/Fs, adsorption to organic (primarily) and inorganic particles defines the fate and transport of these compounds in the estuarine environment.

Sediment transport and sedimentation are the dominant processes that determine the fate of PCBs in OU1 (Black & Veatch, 2011). Because Aroclor 1268 and PCDD/Fs exhibit similar physical-chemical properties and were released to the marsh associated with the same source, PCDD/Fs are expected to adhere to the same fate and transport processes as Aroclor 1268 and be co-located with Aroclor 1268.

2.5 Distribution of Aroclor 1268 and PCDD/F in OU1 Sediments

The distribution of Aroclor 1268 and PCDD/F in the OU1 sediments is consistent with the CSM presented in the preceding sections. Figure 4 shows the original Aroclor 1268 concentration distribution from sediment sampling conducted across OU1 prior to the 1998-99 removal response action. The Aroclor 1268 distribution shows the highest condition bordering the Domain 1 shoreline and upper reach of the Main Canal. A high degree of spatial attenuation is expressed east to west across the Domain 1 marsh flats, and to the south along the shoreline owing to the dense vegetation of the marsh flats. A more moderate degree of spatial attenuation is expressed in the tidal channels, whether in the Main Canal (east to west) or in Eastern Creek (north to south). A similar distribution pattern is exhibited for the pre-removal PCDD/F condition, expressed as the dioxin TEQ value[1] (Figure 5). Table 1a provides a summary of paired PCDD/F congeners and Aroclor 1268 historical sampling results.

[1] PCDD/F congener data are commonly evaluated as a single result, where each congener concentration is normalized to the congener 2,3,7,8-TCDD using congener-specific toxicity equivalency factors ("TEFs") (van den Berg *et al.*, 2006) and the values are summed to generate a PCDD/F TEQ value. The present TEF scheme is based on 2005 values reported by the World Health Organization.

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2.5.1 PCDD/F Homologue Profiles

2.5.1.1 Overview

A simple histogram graphical representation of the 10 PCDD/F homologue classes can used to illustrate the "chemical fingerprint" or profile of the PCDD/F condition. This method of data analysis can be used to identify commonality (or lack thereof) of the source of PCDD/F to individual sample sites from the study area. PCDD/F congener profiling of historical sediment samples collected in the vicinity of the Site and in the regional vicinity of Brunswick, Georgia reveal two distinct PCDD/F congener patterns: (i) a PCDF-dominant profile consistent with byproducts of the chlor-alkali process (Kannan *et al.*, 1997; Rappe et al., 1991; and Yamamoto *et al.*, 2017[2]), and (ii) a PCDD-dominant profile associated with the regional condition.

PCDD/F profiles were created from the five PCDD and five PCDF congener groups (see table below) as a compositional percentage of the total congeners concentration for a given sample.

Dioxin Congeners	Total HpCDDs	Total HxCDDs	OCDD	Total PeCDDs	Total TCDDs
Furan Congeners	Total HpCDFs	Total HxCDFs	OCDF	Total PeCDFs	Total TCDFs

Profiles characterized from upland soils, Turtle River/regional sediments, and LCP marsh sediments are discussed in the following sections. Table 1b provides the PCDD/F homologue results from these prior sampling events.

2.5.1.2 Upland Profile

Two soil samples from Sprenger *et al.* (1997) and one soil sample from Kannan *et al.* (1997) capture the upland soil condition prior to the 1995-1997 upland removal action. These samples exhibit a strong PCDF signature (as shown in Chart 1 below) consistent with the historical byproducts of the chlor-alkali process and may be used for comparison with patterns measured in OU1 sediment samples.

[2] In the Yamanoto et al. study, exclusively PCDD/Fs were formed in tests using graphite electrodes.

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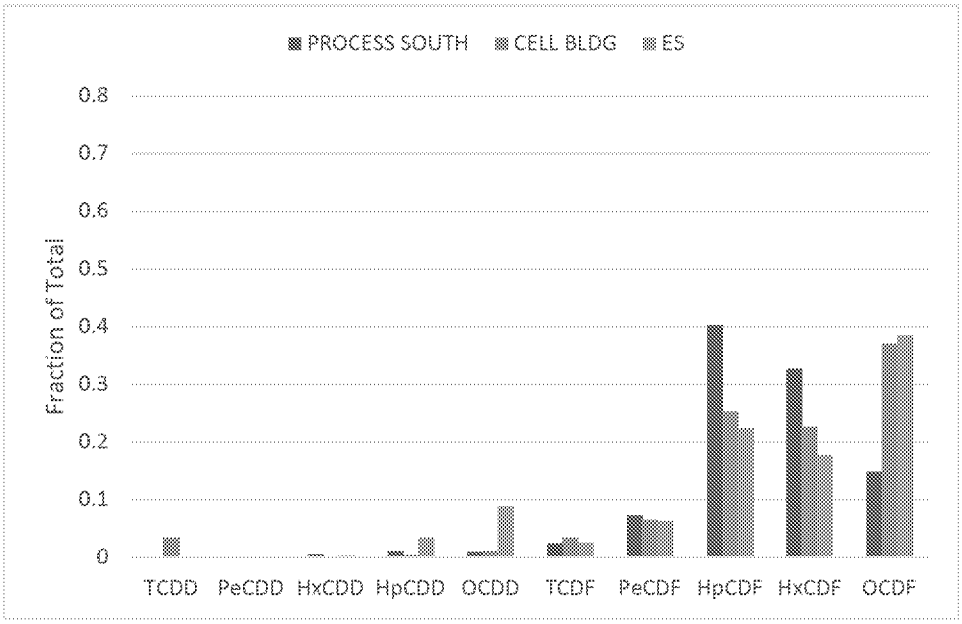

Chart 1. PCDD/F homologue profiles for upland soil samples

2.5.1.3 Turtle River/Regional Profile

A regional-based study known as the "Brunswick Initiative", a collaborative effort involving USEPA and the Georgia Environmental Protection Division ("EPD"), included collection and testing of sediment samples within the Turtle River Estuary, St. Simons Sounds, and areas east of the Brunswick Peninsula. The homologue patterns reveal a PCDD-dominated profile comprised mostly of OCDD followed by HpCDD and HxCDD homologue groups.

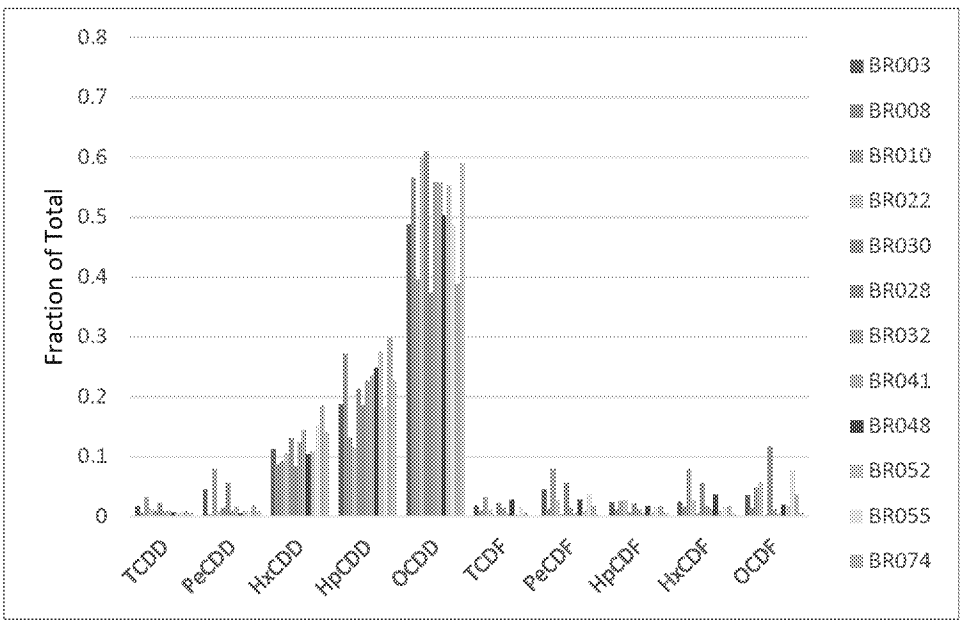

Chart 2. PCDD/F homologe profiles for samples collected during Brunswick Initiative Study

2.5.1.4 LCP Marsh (OU1)

Sediment samples collected by USEPA from 1995-1996 and CDR and Geosyntec (2001) characterize the condition in OU1. Homologue profiles for these samples are provided below (Charts 3 and 4). Profiles for samples collected proximate to the Outfall Pond former discharge point exhibit a strong PCDF pattern mixed with similar concentration of OCDD and HpCDD homologue groups, suggesting a mixed environment of Site-related and regional influences. Further afield in OU1 (Purvis Creek and Western Creek Complex sample locations), the pattern shifts further to a dominant PCDD profile similar to the regional condition. The shift from the PCDF to PCDD profile along the concentration gradient suggests that Site influence diminishes to the regional condition further into OU1. Figure 6 illustrates the spatial relationship of the past PCDD/F sampling results in terms of the homologue profile pattern shift from the uplands (source) across OU1 (mixed environment).

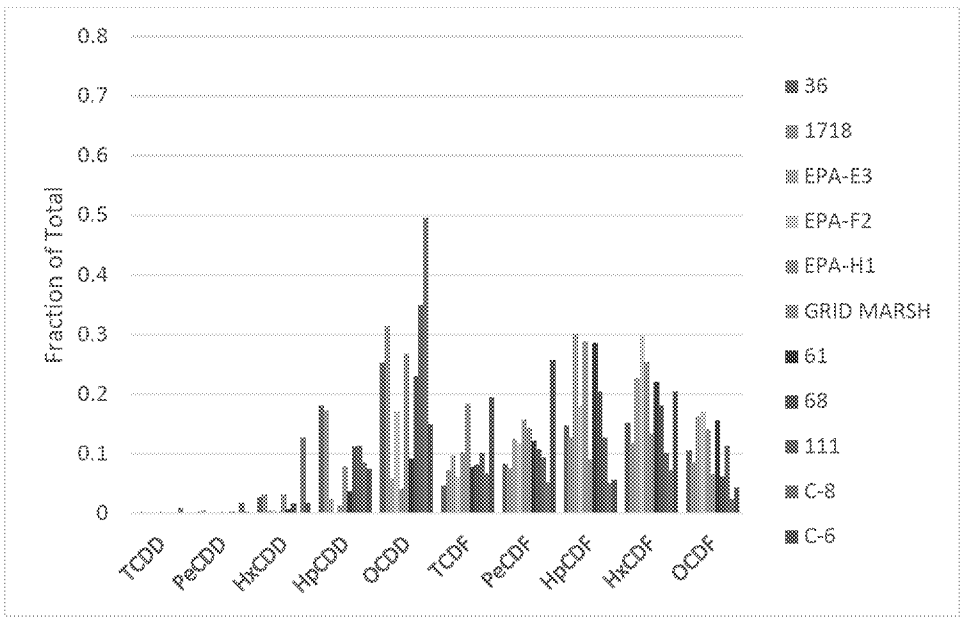

Chart 3. PCDD/F homologue profiles for Domain 1 and associated tidal channels (Eastern Creek and Main Canal).

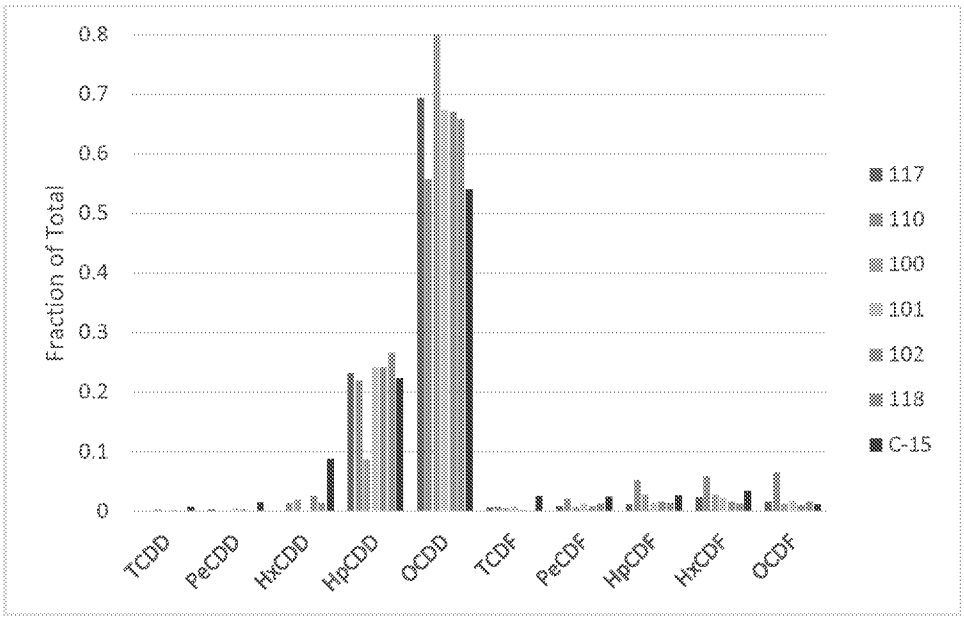

Chart 4. PCDD/F homologue profiles for samples collected from Purvis Creek and Western Creek Complex.

2.6 1998-99 OU1 Removal Action

From 1998 to 1999, approximately 13 acres of marsh flats in the near-shore area of Domain 1 were excavated, backfilled, and revegetated with indigenous marsh grasses (Figure 7). Dredging was also performed in a portion of Eastern Creek and the Main Canal. Some of the current co-location sampling was performed in the removal action areas, and it should be expected that dioxin congener profiles (and TEQ concentration) have been altered in comparison to the pre-removal condition representations presented in prior sections of this report. These elements are considered in the data evaluation section presented later in this report.

3 SAMPLING LOCATIONS FOR CO-LOCATION STUDY SUPPORT

Surficial sediment (*i.e.*, upper 6 inches) sampling for the co-location study was performed at 14 areas, 28 total locations, in accordance with the EPA-approved Work Plan. Sampling areas targeted the planned OU1 Remedial Action areas, with a greater sampling density toward historical sediment sampling locations that exhibited a more dominant PCDF congener profile indicative of a greater level of Site-related contribution. Sampling locations are summarized below and illustrated on Figure 8:

- Thin-layer cover Remedial Action areas (south of the causeway)
  - one sampling area on the marsh flats flanking the causeway at the upper end of the Main Canal (D1-1)
  - one sampling area on the marsh flats between the 13-acre removal action area and Eastern Creek (D1-2)
  - one sampling area at the south end of Eastern Creek on the marsh flats to the west (D2-1)
- Dredging Remedial Action areas
  - three sampling areas within the Main Canal (MC-1, MC-2, MC-3)
    - of these, areas MC-1 and MC-2 are in areas of the former Removal Action dredging
  - four sampling areas within Eastern Creek (EC-1, EC-2, EC-3, EC-4)
    - of these, areas EC-1 and EC-2 are in areas of the former Removal Action dredging, area EC-3 at the approximate terminating point of that dredging, and area EC-4 beyond the former dredging limits
- Capping Remedial Action areas
  - one sampling area in each of three portions of Purvis Creek designated for remedial action (PC-1, PC-2, PC-3)
  - one sampling area in Domain 3 Creek[3] (LC-1).

Each sampling area consisted of two adjacent, 5-foot by 5-foot sub-areas, resulting in two independent samples at each sampling area (*e.g.*, D1-1A and D1-1B for area D1-1). Each sample was collected as a composite of sediment (from 5 points[4]) within each sub-area from a depth interval of approximately 0-6 inches. The sample units that make up each composite were homogenized in a stainless-steel bowl prior to transfer to the sampling container. Sediments from marsh flats were collected using a stainless-steel spoon. Sediments from Purvis Creek and smaller tidal channels of the LCP marsh were collected using a hand auger. Clean (decontaminated)

[3] This portion of the Domain 3 Creek feature has been referred to as "Landfill Creek" is some of the past documents.
[4] At times additional sub-sampling points were necessary, owing to hard substrate and minimal sample recovery.

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sampling equipment was used to collect each sample (*i.e.*, two sets of clean sampling equipment were used per sampling area).

All samples were labeled, placed on ice in a cooler, and logged under standard chain of custody. Sediment samples for PCB Aroclor characterization were shipped to Alpha Analytical Services in Mansfield, Massachusetts and analyzed by SW-846 Method 8082A. Sediment samples for PCDD/F characterization were shipped to SGS AXYS Analytical Services, Inc. in Sidney, British Columbia and analyzed by SW-846 Method 8290A.

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4 RESULTS

4.1 Paired Aroclor 1268 and Dioxin TEQ Results

Aroclor 1268 concentrations in sediment are mapped in Figure 9[5]. Concentrations ranged from 0.604 milligrams per kilogram[6] ("mg/kg") (PC-3B) to 31.1 mg/kg (PC-1A) with the highest results occurring in the southern-most locations in Eastern Creek (EC-3A, EC-3B, EC-4A) and Purvis Creek north of the causeway (PC-1A, PC-1B). Dioxin TEQs in sediment ranged from 6.88 nanograms per kilogram[7] ("ng/kg") (PC-3B) to 863 ng/kg (EC-3B).

Figure 9 also posts the PCDD and PCDF results in terms of the mass concentration, as well as the total dioxin TEQ (a representation of relative toxicity, not concentration). PCDD/F mass distribution exhibits a similar spatial profile to Aroclor 1268 with the highest concentration occurring at the southern-most locations in Eastern Creek (EC-3A, EC-3B, EC-4A, EC-4B), and Purvis Creek north of the causeway (PC-1A, PC-1B), as shown on Figure 9.

The spatial distributions of Aroclor 1268 and PCDD/F validate the CSM. Both constituents exhibit moderate concentration in the Domain 1 areas where previous Removal Response dredging had occurred, and more elevated concentration in the Domain 1 areas further afield in the upper reaches of Eastern Creek where past dredging has not taken place (*i.e.*, the original condition remains).

Table 2a provides the summary of PCDD/F congener and Aroclor 1268 sampling results. Appendix A provides the complete laboratory reports for the co-location study.

4.2 Dioxin TEQ Relative to Preliminary Remedial Goal

The ROD presented a preliminary remedial goal ("PRG") for dioxin TEQ at 260 ng/kg, stating this as a "conservative-based remedial goal". Sampling results are therefore compared herein to this PRG value. Sampling sites exceeding the PRG are as follows:

Location	Dioxin TEQ (ppt)	Aroclor 1268 (ppm)
PC-1A	381	31.1
PC-1B	121	24.5
EC-3A	135	24.4
EC-3B	863	22.1
EC-4A	736	28.8
EC-4B	124	7.7

[5] Sediment from two sample locations contained additional PCBs. Sample D1-2A reported Aroclor 1016 at 0.06 mg/kg, Aroclor 1232 at 0.09 mg/kg, and Aroclor 1260 at 0.93 mg/kg in addition to Aroclor 1268 at 1.37 mg/kg. Sample EC-1A reported Aroclor 1242 at 0.25 mg/kg in addition to Aroclor 1268 at 12.6 mg/kg.

[6] Also known as parts per million ("ppm").

[7] Also known as parts per trillion ("ppt").

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4.3 PCDD/F Congener Profiles

PCDD/F homologue profile pie charts for the co-location samples are shown in Figure 10. Similar PCDD-dominant profile patterns are exhibited across the Main Canal, Domain 1 and 2 marsh flats, and proximate Purvis Creek locations – the PCDF composition at these locations comprises generally 0.1 (10%) of the total PCDD/F composition. OCDD is the predominant homologue group detected comprising about 0.5 (50%) of the total PCDD/F composition. A stronger PCDF profile (comprising approximately 0.3-0.4 (30-40%) of the total PCDD/F composition, is exhibited at the upper reach of Eastern Creek, which is consistent with the CSM as this area is beyond the limits of the past dredging conducted at the Site and retains the original chlor-alkali influenced signature.

Table 2b is a summary of PCDD/F homologue results.

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5 STATISTICAL EVALUATION

5.1 Co-location Evaluation Methods

5.1.1 Regression Analysis

5.1.1.1 Interpretation of the Regression Analysis

An ordinary least-squares ("OLS") regression analysis estimates a linear model that predicts the dependent variable value as a function of a single independent variable. Three key outputs of the regression analysis are the slope, coefficient of determination, and calculated probability, which are summarized as follows:

- **Slope**. The slope of the regression line (m) represents the rate of change in the dependent variable as the independent variable changes. A slope greater than 0 indicates a positive correlation (*i.e.*, both variables move in tandem). Conversely, a slope less than 0 indicates a negative correlation (*i.e.*, one variable increases as the other decreases). A slope of 0 indicates no correlation.
- **Coefficient of Determination.** The coefficient of determination (R^2) measures the variation in the dependent variable data explained by the model (*i.e.*, how well the linear regression fits the data set). R^2 ranges from 0 to 1 where 0 indicates that the model explains none of the variability and 1 indicates that the model explains all the variability.
- **Calculated Probability.** The calculated probability (p-value) provides insight into whether the mathematical relationship derived for the sample data potentially exists in the larger population. The calculated probability tests the null hypothesis that the independent variable is not correlated with the dependent variable. If the calculated probability is less than the significance level (typically set at 5% or 0.05), the sample data provide sufficient evidence to reject the null hypothesis for the entire population.

5.1.1.2 General Assumptions of Regression Analysis

According to the Gauss-Markov theorem, the OLS estimates are each a "best linear unbiased estimate" (*i.e.*, are unbiased and have the least amount of variance) of the respective population parameters when the general assumptions described below hold true. Calculations and visual aids (charts) for testing select assumptions are provided in Appendix B.

- **Zero Conditional Mean of Errors.** The unconditional mean of the population values of the random error term equals zero, *i.e.*, the residual error around the regression line is expected to be zero given any values of the independent variable. This assumption is examined by a plot of the residuals versus the independent variable (Aroclor-1268 concentration). If the residual errors are uncorrelated with Aroclor-1268 concentration, then the assumption is satisfied. All cases of co-location evaluated in Section 5.2 meet this condition (see Appendix B).

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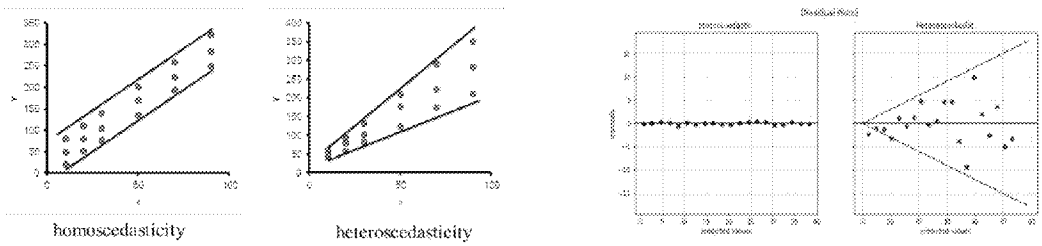
- **Independence of Errors.** The distribution of errors is random and not influenced by or correlated to the errors in prior observations. This assumption holds true for singular and pooled cross-sectional data sets (*i.e.*, random sampling performed for one event or multiple events at different points in time), such as the data evaluated in this study, as statistical independence of sample observations is implied.
- **Homoscedasticity of Errors.** Variance around the regression line is constant for all values of the independent variable (shown below). Conversely, heteroscedasticity is present when the magnitude of error differs across values of the independent variable.



Homoscedasticity in a linear regression model can be tested using the Breusch-Pagan ("BP") Test, which calculates outputs of the OLS analysis (slope, coefficient of determination, and p-value) from an auxiliary regression of the squared residuals ($\hat{u}^2$) on the independent variables. If the test statistic has a p-value below an appropriate threshold ($p<0.05$) then the null hypothesis of homoscedasticity is rejected, and heteroscedasticity is assumed. White's Test for homoscedasticity was also utilized in this analysis to confirm the results of the BP Test. White's test relaxes the assumption of normality (Baum, 2006) and allows the independent variable to have a nonlinear effect on the error variance. The calculation is performed similar to the BP method, with outputs of the OLS analysis calculated from an auxiliary univariate quadratic polynomial of the squared residuals on the independent variables ($\hat{Y}^2$, $\hat{Y}$). Similar to the BP Test, if the test statistic has a p-value below an appropriate threshold ($p<0.05$) then the null hypothesis of homoscedasticity is rejected, and heteroscedasticity is assumed. Calculations testing the presence of homoscedasticity for each case of co-location evaluation are included in Appendix B.

The presence of heteroscedasticity in a data set causes bias in the estimates of variance of the coefficients, and thus increases the probability of making a Type I or Type II error in hypothesis testing. In the context of this study, the regression may indicate PCDD/F is correlated with Aroclor 1268 concentration when it is in fact not (Type I error) or may incorrectly indicate that PCDD/F is not correlated with Aroclor 1268 concentration (Type II error). It is important to note that only severe heteroscedasticity may jeopardize the conclusions of the hypothesis testing. As common rule of thumb, a ratio of the generalized least square (*e.g.*, weighted least squares (see Section 5.1.1.3)) and OLS error variance[8] exceeding 10 indicates "severe heteroscedasticity" (Fox, 1997). Additionally, regression analysis using heteroscedastic data will still provide an unbiased estimate for the relationship between the predictor variable and the outcome (Kleinbaum, 1998).

[8] The higher of the two values acts as the numerator.

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Data points with large residuals (outliers) and/or high leverage (*i.e.*, extreme/outlying values of the independent variable) (see Section 5.1.1.4 on Cook's Distance analysis) were removed to mitigate heteroscedasticity and justify the conclusions from hypothesis testing for the raw linear regression. Data transformation was considered as a method to mitigate heteroscedasticity; however, data transformations fundamentally transform the nature of the variable to which they are applied and may not address the hypothesis of interest regarding the original data (Feng et al. 2014; Osborne, 2002). Consequently, data transformations were not utilized in the regression analysis.

- **Normality of Errors.** The assumption of normality of errors is not necessary in linear regression analysis of sufficiently large sample size (Schmidt and Finan, 2018; Lumley et al, 2002) due to the central limit theorem, which implies that the sampling distribution of the coefficients will approach a normal distribution as sample size grows larger. A minimum sample size "sufficiently large" is commonly considered to be from greater than 10 (Schmidt and Finan, 2018) to greater than 20 (Stevens, 2009) times the number of observed parameters, or conservatively 20 samples for a simple linear regression. All cases of co-location (including those that exclude outliers) exceed a sample count of 20, thus the assumption of normality is not necessary for the regression analysis.

5.1.1.3 Weighted Least Squares Analysis

The method of weighted least squares ("WLS") is an extension of OLS regression that minimizes the sum of weighted squared residuals to produce homoscedasticity. Weights that provide the expected and desired statistical properties require a priori information regarding the parameters (Tellinghuisen, 1996); however, it is common practice to calculate weights as the reciprocal of a squared predictor based on an auxiliary regression of the absolute value of the residuals on the independent variables. WLS regression was performed by using the "Real Statistics" (Excel Add-In) WLS data analysis tool.

5.1.1.4 Cook's Distance Analysis

Cook's Distance analysis estimates the influence of data point on the fitted response values of the linear regression and is useful for identifying outliers and/or high leverage points. Cook's Distance for an observation is calculated using the following equation:

$$D_i = \frac{\hat{u}_i^2}{p\,MSE}\left(\frac{h_{ii}}{(1-h_{ii})^2}\right)$$

where MSE is the mean squared error, p is the number of coefficients in the regression model, $\hat{u}_i$ is the *i*th residual, and h_{ii} is the *i*th leverage value.

Observations scoring a Cook's Distance value above 4/n (where n is the number of observations in the data set) were considered outliers and/or exert high leverage (Bollen and Jackman, 1990; Van der Meeer anvd Pelzer, 2010). It is important to note that these observations are not necessarily erroneous, and therefore should not be discarded on the basis of an outlier test (EPA, 1992). Accordingly, linear regression and statistical measures of association (discussed in Section 5.1.2) were performed for each case of co-location including and excluding outlier observations, and the results were assessed collectively.

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See Appendix C for Cook's Distance calculations.

5.1.2 Statistical Measures of Association

Statistical measures of association define the strength of the relationship or level of association between two variables in terms of the degree of monotonicity (*i.e.*, entirely increasing or decreasing). This is measured by the coefficient of correlation (R) where:

- R of +1 indicates a perfect monotonically increasing relationship;
- R of -1 indicates a perfect monotonically decreasing relationship; and
- R of 0 indicates that the relationship is not monotonic.

An R approaching +1 (monotonically increasing relationship) or -1 (monotonically decreasing relationship) indicates strong association between variables, whereas an R approaching 0 indicates weak association between variables. In the context of co-location, an R approaching +1 specifies strong association between Aroclor 1268 and PCDD/F where samples characterized by elevated Aroclor 1268 are expected to also exhibit elevated concentrations of PCDD/F and thus, suggests a high degree of co-location. The measures of association considered for evaluation of co-location are described below:

- Pearson Correlation - A parametric measure of linear correlation between two variables. Pearson's correlation coefficient (r_p) is calculated using the following formula:

  $$r_p = \frac{n(\sum x_i y_i) - \sum x_i \sum y_i}{\sqrt{(n\sum x_i{}^2 - (\sum x_i)^2)\,(n\sum y_i{}^2 - (\sum y_i)^2)}}$$

  where x_i and y_i are the Aroclor 1268 concentration and PCDD/F ~~TEQ~~ for sediment sample *i* and n is the number of samples.

  General assumptions of the Pearson Correlation include linearity and normality of the independent and dependent variable. If these assumptions are not satisfied, it is appropriate to apply a log-transformation to both variables to achieve linearity and normality (Bishara and Hittner, 2012; Rasmussen and Dunlap, 1991).

- Spearman Rank-order Correlation- A nonparametric measure of statistical dependence between rankings of two variables. The Spearman Correlation does not assume variables approximate linearity or normal distribution. Spearman's rank coefficient (r_s) is calculated using the following formula:

  $$r_s = 1 - \frac{6\sum d_i^2}{n(n^2-1)}$$

  where d_i is the difference in rank between Aroclor 1268 concentration and mass concentration of PCDD/F for sediment sample *i* compared to the entire data set and n is the number of samples.

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5.2 Results of the Co-location Analysis

5.2.1 Overview

Co-location of PCDD/F and Aroclor 1268 were evaluated for three cases:

- Case 1 provides an evaluation on co-location of PCDD/F and Aroclor 1268 using exclusively the current 2018 co-location study sampling data set;
- Case 2 provides an evaluation on co-location of PCDD/F and Aroclor 1268 based on the combined historical and current data set for OU1; and
- Case 3 examines the paired PCDD/F and Aroclor 1268 condition in a data set comprised locations not altered by the past Removal Action – thus, the 2018 sampling locations in the Main Canal (MC-1, -2, -3) and lower portion of Eastern Creek (EC-1, -2) were intentionally excluded (this data set, therefore, offers the most representative degree of co-location).

Each case is divided into two parts (an "a" and "b"):

- The 'a' cases provide an assessment of the total PCDD/F mass to Aroclor 1268;
- The 'b' cases provide an assessment of exclusively the PCDF congener mass (believed to be more associated with the chlor-alkali production) to Aroclor 1268.

See Appendix D for complete details regarding the statistical analyses.

5.2.2 Case 1: 2018 Data Set

The results of the statistical analyses for Case 1 are summarized in the table below.

		Case 1a	Case 1a, excl. outliers	Case 1b	Case 1b, excl. outliers
Linear Regression	Homoscedastic	O	X	O	O
	m	721	583	402	295
	R^2	0.58	0.62	0.55	0.62
	p	2.3E-06	5.4E-06	6.0E-06	5.7E-06
Pearson Correlation Analysis	r_p	0.66 (1)	N/A	0.74(1)	0.63(1)
Spearman Rank-order Correlation Analysis	r_s	0.60	0.57	0.73	0.59
	n	28	24	28	24

Notes:
'X' Denotes homoscedasticity of the data set
'N/A' denotes Pearson Correlation not applicable, data sets not normally or lognormally distributed
(1) Denotes log-transformation applied to both variables to satisfy assumptions of Pearson Correlation
O' Denotes that heteroscedasticity is not severe based on ratio of WLS and OLS variance

The data set indicates co-location of total PCDD/F with Aroclor 1268. The linear regression analysis for Case 1a is statistically significant ($p < 0.05$), providing sufficient evidence to reject the null hypothesis that total PCDD/F is not correlated with Aroclor 1268. The linear regression

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analysis shows a positive correlation that explains 58% (including outlier observations) or 62% (excluding outlier observations) of the variation in the total PCDD/F. The Pearson correlation coefficient and Spearman rank-order coefficients for Case 1a indicate moderate increasing monotonicity (association).

Likewise, the data set demonstrates co-location of exclusively PCDF congener mass with Aroclor-1268 (Figure 11). The linear regression analysis for Case 1b indicates sufficient evidence to reject the null hypothesis that furan homologues are not correlated with the Aroclor 1268 ($p < 0.05$). The linear regression shows a positive correlation that explains 55% (including outlier observations) and 62% (including outlier observations) of the variation in total furan congener mass. The Pearson correlation coefficients and Spearman rank-order coefficients for Case 1b indicate strong increasing monotonicity (association).

5.2.3 Case 2: Combined Historical and Current Data Sets

The results of the statistical analyses for Case 2a and 2b are summarized in the table below.

		Case 2a	Case 2a, excl. outliers	Case 2b	Case 2b, excl. outliers
Linear Regression	Homoscedastic	O	X	O	X
	m	97.5	90.4	92.1	79.7
	R^2	0.87	0.80	0.87	0.86
	p	6.1E-21	2.6E-16	5.8E-21	1.9E-19
Pearson Correlation Analysis	r_p	N/A	0.75(1)	N/A	0.79(1)
Spearman Rank-order Correlation Analysis	r_s	0.71	0.66	0.80	0.77
	n	46	44	46	44

Notes:

'X' Denotes homoscedasticity of the data set

'N/A' denotes Pearson Correlation not applicable, data sets not normally or lognormally distributed

(1) Denotes log-transformation applied to both variables to satisfy assumptions of Pearson Correlation

O' Denotes that heteroscedasticity is not severe based on ratio of WLS and OLS variance

The addition of the historical samples to the current data set caused the Pearson correlation coefficients and Spearman rank-order coefficients to increase (approach +1), indicating a higher degree of co-location from Case 1 to 2. In addition, the regression analysis for Cases 2a and 2b exhibits greater statistical significance than that of their Case 1 counterpart. The regression analysis yields similar results for Cases 2a and 2b: a positive correlation expressed as a linear function that explains above 80% of the variation in the dependent variable (total PCDD/F in Case 2a and total furan homologues in Case 2b).

5.2.4 Case 3: Unaltered (Outside of 1998-99 Removal Action) Areas of OU1

The results of the statistical analyses for Cases 3a and 3b are summarized in the table below.

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		Case 3a	Case 3a, excl. outliers	Case 3b	Case 3b, excl. outliers
Linear Regression	Homoscedastic	O	X	O	X
	m	97.2	89.2	91.8	78.5
	R^2	0.86	0.80	0.87	0.86
	p	5.9E-15	1.4E-11	5.8E-15	8.6E-14
Pearson Correlation Analysis	r_p	0.85(1)	0.78(1)	0.87(1)	0.82(1)
Spearman Rank-order Correlation Analysis	r_s	0.78	0.74	0.83	0.79
	n	33	31	33	31

Notes: 'X' Denotes homoscedasticity of the data set

'N/A' denotes Pearson Correlation not applicable, data sets not normally or lognormally distributed

(1) Denotes log-transformation applied to both variables to satisfy assumptions of Pearson Correlation

O' Denotes that heteroscedasticity is not severe based on ratio of WLS and OLS variance

The data set indicates a high degree of co-location of total PCDD/F with Aroclor 1268. The linear regression analysis for Case 3a is statistically significant ($p < 0.05$) providing sufficient evidence to reject the null hypothesis that total PCDD/F is not correlated with Aroclor 1268 concentration. The linear regression analysis shows a positive correlation that explains 86% (including outlier observations) or 80% (excluding outlier observations) of the variation in the total PCDD/F. The Pearson correlation coefficient and Spearman rank-order coefficient for Case 3a indicate strong increasing monotonicity (association), higher than other cases previously considered.

Likwise, the data set demonstrates a high degree of furan congener mass co-location with Aroclor 1268. The regressions analysis for Case 3b shows a positive correlation and provides sufficient evidence to reject the null hypothesis that furan homologues are not correlated with the Aroclor 1268 ($p < 0.05$). The linear regression explains approximately 86% of the variation in total furan homologues. The Pearson correlation coefficients and Spearman rank-order coefficients for Case 3b indicate strong increasing monotonicity (association).

5.3 95% UCL of PCDD/F TEQ

The upper 95% confidence level on the mean concentration ("95% UCL") was computed for PCDD/F TEQ from the co-location study data set as a mode of comparison to the PRG presented in the ROD. The 95% UCL is customary to comparing results to a risk-based criterion. The 95% UCL was calculated using the EPA's ProUCL software (version 5.1). ProUCL input and output is presented in Appendix E. The 95% UCL for PCDD/F TEQ in sediment is 200 ng/kg, which is below the PRG of 260 ng/kg.

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6 SUMMARY AND CONCLUSION

The 2018 study involved strategic sampling targeting the various portions of OU1 designated for Remedial Action, contributing numerous additional characterization points in OU1 to supplement prior OU1 sampling for paired Aroclor 1268 and PCDD/F testing. In doing so and based on the collaborating results of the 2018 co-location study, the CSM developed in 2014 by the USEPA is further validated.

The statistical evaluation provides clear and meaningful evidence of the strong association of PCDD/F with Aroclor 1268 in the OU1 sediments. This allows the following factors to support the conclusions developed from the Aroclor 1268 characterization in OU1, to be applied to PCDD/F, and no further assessment is necessary.

1. The paired test results support the CSM regarding co-location, and thus remediating the PCB condition will remediate a similar PCDD/F condition.
2. The highest PCDD/F condition occurs in the portion of Eastern Creek beyond the area of the past Removal Action dredging, where the highest condition in Eastern Creek should be expected (according to the CSM).
3. It is well documented that the tidal channel sediments exhibit a significantly higher contaminant condition relative to the adjoining marsh flats. Remediation of the full extent of Eastern Creek in the OU1 Remedial Action will address the elevated dioxin TEQ present in that channel.

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TABLES

Table 1a. Historical Sampling PCDD/F Congeners and Aroclor 1268 Results

	OCDD (ng/kg)	1234678HpCDD (ng/kg)	123478HxCDD (ng/kg)	123678HxCDD (ng/kg)	123789HxCDD (ng/kg)	12378PeCDD (ng/kg)	2378TCDD (ng/kg)
TEF	0.0003	0.01	0.1	0.1	0.1	1	1
1718	5770	798	41.4	13.4	30.1	4.9	7.8
36	6850	1130	12.8	92.7	49.8	4.9	15.9
61	13100	2140	42.6	57.3	38.9	8.6	29.3
68	14800	2140	24.3	48.7	48.2	7.7	20.6
100	1700	170	1.2	0.75	0.90	0.55	0.38
101	1387	125	2.3	1.4	1.7	0.97	0.77
102	1795	176	0.827	5.7	9.9	0.50	0.21
110	690	66	0.46	0.3	0.3	0.44	0.17
111	3286	357	11.7	7.4	8.5	3.6	1.45
117	1481	137.8	2.6	1.65	1.913	1.5	0.78
118	1803	184.2	2.8	1.8	2.1	2.3	1.47
BR048	1500	190.0	3.1	8.1	11	6	4.0
C-15	5860	610	34.2	24.4	43.0	7.2	5.7
C-6	8810	891	11.4	24.2	40.9	6.2	53.7
C-8	5280	597	5.0	320.0	53.0	8.70	13.4
EPA-E3	14000	2410	48.8	52.5	50.6	12.2	14.6
EPA-F2	20700	2420	49	503.0	192.0	15.5	1.0
EPA-H1	22000	3480	61.1	91.6	54.4	15.40	7.3
GRID MARSH	1600	170	4.0	8.9	8.2	0.8	7.4
BR003	65	10	6.0	6.0	6.0	6.0	2.5
BR008	1500	160	2.2	5.1	7.0	1.5	4.0
BR010	30	6	6.0	6.0	6.0	6.0	2.5
BR022	130	10	6.0	6.0	6.0	6.0	2.5
BR028	40	6	6.0	6.0	6.0	6.0	2.5
BR030	2600	250	5.2	9.2	19.0	3.3	1.1
BR032	2700	310	5.1	11.0	20.0	2.9	3.8
BR041	1700	190	4.1	7.7	15.0	2.4	1.1
BR052	380	20	6.0	1.8	3.6	6.0	2.5
BR055	80	10	6.0	6.0	6.0	6.0	2.5
BR074	130	15	6.0	6.0	2.4	6.0	2.5
BR080	750	76	1.4	3.1	6.6	6.0	2.5
105	1700	170	0.6	7.5	8.2	0.6	2.0
106	1700	150	1.0	4.0	8.7	0.9	0.3
107	450	44	1.5	0.9	1.1	1.9	0.8
108	710	76	2.7	2.5	6.8	0.4	0.2
CELL BLDG	380	56	5.0	5.2	1.8	0.4	2.2
PROCESS SOUTH	370	110	13.0	6.8	5.0	1.4	1.5

	OCDF (ng/kg)	1234678HpCDF (ng/kg)	1234789HpCDF (ng/kg)	123478HxCDF (ng/kg)	123678HxCDF (ng/kg)	123789HxCDF (ng/kg)	234678HxCDF (ng/kg)	12378PeCDF (ng/kg)	23478PeCDF (ng/kg)	2378TCDF (ng/kg)	PCDD/F TEQ (ng/kg)	Aroclor 1268 (mg/kg)
TEF	0.0003	0.01	0.01	0.1	0.1	0.1	0.1	0.03	0.3	0.1		
1718	1560	1210	187	700	192	15.9	120	293	106	250	214	56.0
36	2870	2000	372	1370	413	33.0	185	676	209	359	393	55.0
61	22200	21000	3800	11900	2770	270	600	5050	1670	2300	2768	1300
68	3960	4860	608	2640	734	387	384	1240	401	682	762	330
100	200	140	24.0	110	17	3.7	9.3	24.0	6.8	6.5	22.5	1.1
101	38.5	29.7	1.5	11.8	2.0	3.0	3.0	0.69	0.69	0.86	6.6	0.09
102	28.6	36.5	6.9	12.1	1.1	2.0	3.9	0.41	0.42	2.8	7.4	0.13
110	11.0	21.0	0.29	8.0	0.2	0.36	0.31	0.35	0.36	0.4	2.8	0.25
111	1062.3	1101.1	97	479	139	5.5	141.4	170	53.2	154	138	6.1
117	34.9	26.1	2.713	12.1	0.99	1.5	1.5	0.75	0.8	0.85	6.9	11
118	46.4	38.7	2.551	8.7	2.153	3.3	3.2	0.84	0.8435	1.8	9.4	10.00
BR048	58.0	37.0	3.4	10	4.6	6.0	7.4	6.2	4.60	10	20.4	1.4
C-15	128	145	9.9	68.0	17.8	0.1	27.5	31.9	18.7	32.3	53.6	0.1
C-6	2570	1520	799	5860	1650	328	731	6660	1020	4120	1878	7.6
C-8	260	277	35.10	188	46.5	6.5	48.9	98.5	35.5	104	124	2.20
EPA-E3	39100	43500	6050	20800	5640	349	3020	7280.0	2590	3510	4905	3800.00
EPA-F2	21800	25700	3000	21900	2900	204	2070	5400	1840	1300	3966	1188.00
EPA-H1	75900	92200	15700	49300	15700	661	7790	26100	6100	9660	12111	4000.00
GRID MARSH	390	260	50.0	240	61.0	53.0	52.0	170	120	220	119	6.10
BR003	4.8	2.7	6.0	6.0	6.0	6.0	6.0	6.0	6.0	2.5	15.1	0.01
BR008	38.0	25.0	6.0	10.0	3.2	6.0	3.5	5.2	2.9	10	13.6	0.59
BR010	3.7	1.7	6.0	6.0	6.0	6.0	6.0	6.0	6.0	2.5	15.1	0.05
BR022	12.5	6.0	6.0	6.0	6.0	6.0	6.0	6.0	6.0	2.5	15.2	0.05
BR028	12.5	2.0	6.0	6.0	6.0	6.0	6.0	6.0	6.0	2.5	15.1	0.25
BR030	13.0	12.0	6.0	6.0	6.0	6.0	1.8	6.0	6.0	2.5	15.4	0.11
BR032	60.0	43.0	3.0	10.0	3.9	6.0	6.7	5.1	4.0	10	19.7	0.61
BR041	16.0	15.0	6.0	4.4	2.4	6.0	3.0	6.0	1.3	2.5	11.2	0.12
BR052	12.5	1.6	6.0	6.0	6.0	6.0	6.0	6.0	6.0	2.5	14.7	0.10
BR055	12.5	2.2	2.2	6.0	6.0	6.0	6.0	6.0	6.0	2.5	15.1	0.25
BR074	12.5	6.0	6.0	6.0	6.0	6.0	6.0	6.0	6.0	2.5	14.9	0.04
BR080	7.8	5.9	6.0	2.0	6.0	6.0	6.0	6.0	6.0	2.5	14.9	0.05
105	20.0	34.0	0.3	9.7	1.7	0.6	0.5	0.5	0.6	3.9	8.6	0.99
106	18.0	21.0	0.7	5.7	0.7	1.1	1.0	0.4	0.4	1.9	5.9	0.16
107	0.9	0.6	0.8	0.7	0.4	0.7	0.6	1.3	1.3	0.55	4.3	0.58
108	3.0	3.5	0.6	1.3	0.2	0.3	0.3	0.2	0.3	0.135	3.1	0.60
CELL BLDG	4100	1700	340	1200	280	99.0	120	190	110	99.0	245	53.00
PROCESS SOUTH	5900	12000	340	3400	440	71.0	1300	130	340	53.0	764	450.00

Notes:

HpCDD Heptachlorodibenzo-p-dioxin
HxCDD Hexachlorodibenzo-p-dioxin
PeCDD Pentachlorodibenzo-p-dioxin
OCDD Octachlorodibenzo-p-dioxin
TCDD Tetrachlorodibenzo-p-dioxin
HpCDF Heptachlorodibenzofuran
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OCDF Octachlorodibenzofuran
TCDF Tetrachlorodibenzofuran
TEQ Toxicity Equivalence
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TEF Source: Berg et al Berg, Martin Van Den, et al. "The 2005 World Health Organization Reevaluation of Human and Mammalian Toxic Equivalency Factors for Dioxins and Dioxin-Like Compounds." Toxicological Sciences, vol. 93, no. 2, 2006, pp. 223–241., doi:10.1093/toxsci/kfl055.

Table 1b. Historical Sampling: Total PCDD/F Homologue Results

Location	Total OCDF (ng/kg)	Total HpCDF (ng/kg)	Total HxCDF (ng/kg)	Total PeCDF (ng/kg)	Total TCDF (ng/kg)	Total OCDD (ng/kg)	Total HpCDD (ng/kg)	Total HxCDD (ng/kg)	Total PeCDD (ng/kg)	Total TCDD (ng/kg)	Total Furans (ng/kg)	Total Homologues (ng/kg)
OU1 Locations												
1718	1560	2330	2160	1380	1320	5770	3170	588	81.4	49.8	8750	18409
36	2870	3992	4099	2262	1245	6850	4880	713	75.1	51.8	14468	27038
61	22200	40700	31200	17300	11000	13100	5110	968	167	161	122400	141906
68	3960	13160	11600	6890	5240	14800	7210	1040	182	110	40850	64192
100	11	24.0	24.0	6.5	5	690	75.0	17.0	0.00	3.2	71	856
101	38.5	29.7	47.6	26.3	19.0	1387	498	1.4	9.3	0.77	161	2058
102	28.6	43.4	44.8	24.3	6.2	1795	649	70.2	8.8	7.5	147	2678
110	200	160	180	66.0	24	1700	670	43.0	0.00	5.6	630	3049
111	1062	1198	947	883	947	3286	1062	7.4	3.6	1.4	5036	9396
117	34.9	26.1	52.3	20.1	14.3	1481	495	1.649	7.2	0.78	148	2133
118	46.4	38.7	37.5	36.1	1.8	1803	730	40.6	2.3	1.5	161	2738
BR048	58.0	53.0	110.0	85.0	85.0	1500	740	310	18.0	22.0	391	2981
C-15	128	296	371	270	283	5860	2420	963	163	80.0	1348	10834
C-6	2570	3300	12080	15210	11550	8810	4410	987	149	123	44710	59189
C-8	260	541	765	550	710	5280	902	1360	187	99.4	2826	10654
EPA-E3	39100	72200	54400	30200	23300	14000	5890	990	154	94.2	219200	240328
EPA-F2	16000	17000	28000	11000	5700	16000	0.00	380	0	7.7	77700	94088
EPA-H1	75900	155000	137000	84500	55200	22000	7190	1270	58.4	85.8	507600	538204
GRID MARSH	390	540	800	860	1100	1600	470	190	15.0	15.0	3690	5980
Regional Locations												
BR003	4.8	3.2	3.3	6.0	2.5	65.0	25.0	15.0	6.0	2.4		
BR008	38.0	32.0	44.0	32.0	27.0	1500	720	230	11.0	15.0		
BR010	3.7	2.0	6.0	6.0	2.5	30.0	10.0	7.0	6.0	2.5		
BR022	12.5	6.0	6.0	6.0	2.5	130	25.0	23.0	2.1	2.9		
BR028	12.5	2.4	6.0	6.0	2.5	40.0	20.0	9.0	6.0	2.5		
BR030	13.0	31.0	21.0	14.0	11.0	2600	910	560	60.0	38.0		
BR032	60.0	59.0	88.0	71.0	69.0	2700	1100	600	43.0	43.0		
BR041	16.0	20.0	36.0	17.0	16.0	1700	720	440	51.0	30.0		
BR052	12.5	4.4	6.0	6.0	2.5	380	190	75.0	6.8	3.5		
BR055	12.5	2.6	2.6	6.0	2.5	80.0	30.0	25.0	1.5	1.3		
BR074	12.5	6.0	6.0	6.0	2.5	130	100	62.0	6.1	3.2		
BR080	7.8	7.0	6.1	5.4	2.4	750	290	180	13.0	8.1		
105	20.0	39.0	47.0	12.0	27.0	1700	200	58.0	9.3	14.0		
107	0.00	0.00	0.00	0.00	0.00	450	170	150	9.9	9.8		
108	3.0	3.50	6.8	0.00	0.00	710	76.0	49.0	17.0	13.0		
Upland Locations												
CELL BLDG	4100	2800	2500	720	380	120	42.0	4.5	18.0	380		
PROCESS SOUTH	5900	16000	13000	2900	940	370	410	190	19.0	16.0		
ES	82	21.07	16.7	5.96	2.32	8.35	3.23	0.26	0.04*	0.1*		

Notes:

Total homologues are reported from the laboratory report

* 1/2 detection limit

OCDF Octachlorodibenzofuran
HpCDF Heptachlorodibenzofuran
HxCDF Hexachlorodibenzofuran
PeCDF Pentachlorodibenzofuran
TCDF Tetrachlorodibenzofuran
OCDD Octachlorodibenzo-p-dioxin
HpCDD Heptachlorodibenzo-p-dioxin
HxCDD Hexachlorodibenzo-p-dioxin
PeCDD Pentachlorodibenzo-p-dioxin
TCDD Tetrachlorodibenzo-p-dioxin

Table 2a. 2018 Co-location Sampling: PCDD/F Congeners and Aroclor 1268 Results

	OCDD (ng/kg)	1234678HpCDD (ng/kg)	123478HxCDD (ng/kg)	123678HxCDD (ng/kg)	123789HxCDD (ng/kg)	12378PeCDD (ng/kg)	2378TCDD (ng/kg)
TEF	0.0003	0.01	0.1	0.1	0.1	1	1
D1-1A	4420	438	9.5	17.3	25.0	5.5	3.3
D1-1B	4540	490	9.0	18.2	24.9	5.0	3.4
D1-2A	4020	407	9.0	14.8	24.7	4.8	2.8
D1-2B	3590	371	8.5	14.5	22.6	4.6	3.1
D2-1A	4200	448	9.1	18	25.40	5.36	6.79
D2-1B	3540	423	10.1	18.5	24.7	5.89	5.91
EC-1A	4820	450	8.96	15.8	26.6	4.76	4.14
EC-1B	4010	397	7.36	14.3	21.1	3.92	4.67
EC-2A	5110	484	9.02	19.6	26.6	5.25	10.80
EC-2B	2360	183.0	4.3	7.09	15.1	2.41	1.02
EC-3A	3700	349.0	6.8	14.0	22.1	3.87	9.46
EC-3B	6950	653.0	9.75	20.6	29.1	5.52	37.20
EC-4A	6050	595	10.3	20.5	29.7	5.6	41.10
EC-4B	4240	429	8.0	16.5	24.1	4.1	4.7
LC-1A	4550	443.0	5.41	14.7	11.4	2.74	1.8
LC-1B	8520	815	12.1	26.6	21.1	5.18	8.1
MC-1A	5540	512	9.45	17.6	26.1	4.7	5.8
MC-1B	5610	537.0	10.4	20.5	30.2	5.55	5.8
MC-2A	4670.0	446.0	8.1	15.5	23.5	4.2	4.3
MC-2B	4560	459	8.3	16.0	23.6	4.6	7.1
MC-3A	2440.0	245.0	4.1	8.5	11.5	2.1	3.1
MC-3B	2790	284.0	5.0	9.8	14.1	2.7	3.4
PC-1A	20000	1960.0	19.1	60.0	46.4	8.5	23.6
PC-1B	9760	949	11.1	31.5	30.6	5.7	14.0
PC-2A	1890	154	1.8	4.6	7.3	1.0	1.3
PC-2B	2150	218	1.3	7.1	11.6	0.8	0.8
PC-3A	909	87.9	1.6	3.4	4.3	0.9	1.5
PC-3B	615	57.2	1.2	2.1	2.9	0.6	0.8
EPA Split Samples							
D1-1A	2900	320	9.3	16	21	5.6	3.7
D2-1A	4100	450	12	26	26	7.2	24
EC-2B	1100	120	5.2	6.9	13	3.3	1.7
EC-4A	2400	290	9.7	17	18	5.9	39
EC-4B	5400	580	15	24	28	6.2	9.8
LC-1A	4800	490	9	16	12	4.6	2.8
LC-1B	7200	760	15	30	23	5.9	11
MC-3A	2000	210	5	9.1	11	2.7	3.9
MC-3B	2000	220	6.1	11	16	3.1	3.6
PC-1A	6900	810	17	41	35	8.2	19
PC-1B	4200	450	8.6	21	20	5.3	13
PC-2B	1800	190.0	1.0	7.3	12.0	0.85	0.9

	OCDF (ng/kg)	1234678HpCDF (ng/kg)	1234789HpCDF (ng/kg)	123478HxCDF (ng/kg)	123678HxCDF (ng/kg)	123789HxCDF (ng/kg)	234678HxCDF (ng/kg)	12378PeCDF (ng/kg)	23478PeCDF (ng/kg)	2378TCDF (ng/kg)	PCDD/F TEQ (ng/kg)	Aroclor 1268 (mg/kg)
TEF	0.0001	0.01	0.01	0.1	0.1	0.1	0.1	0.03	0.3	0.1		
D1-1A	125	114	12.9	75.1	20.4	1.7	16.7	40.2	16.4	35.3	41.9	2.3
D1-1B	166	168	20.3	110	28.8	2.5	21.5	61.4	21.4	52	51.5	5.1
D1-2A	53.5	56.3	4.18	26.6	7.75	0.698	9.14	13.5	6.87	16.7	26.9	1.37
D1-2B	51.4	62.1	5.06	31.4	8.73	0.708	9.97	15.3	7.85	19.7	27.6	2.29
D2-1A	190	256	28.8	305	97.5	6.48	52.3	215.0	90.0	131	118.7	3.03
D2-1B	124.0	196.0	13.9	145.0	41.2	2.94	47.6	81.00	45.00	68.8	71.0	3.22
EC-1A	90.2	107.0	8.9	63.8	17.9	1.4	16.5	33.80	13.70	36.2	39.9	4.49
EC-1B	90.7	102.0	9.32	65.6	18.8	1.38	14.4	38.30	14.20	46.6	39.2	4.58
EC-2A	162.0	198.0	20.2	159	44.9	3.6	28.6	97.20	33.10	142	80.8	12.6
EC-2B	21	24.2	2.72	18.3	4.9	0.35	3.46	10.5	3.7	11.1	14.1	5.67
EC-3A	344.0	407.0	47.5	402.0	110	9.30	54.8	244.00	77.7	199.00	134.9	24.40
EC-3B	937.0	869.0	248	2640	779	68.40	139	2310	702.00	1520	863.1	22.1
EC-4A	985.0	881.0	251.0	2340.0	691	67.9	133.0	1800.00	574.0	1140.00	735.4	28.8
EC-4B	305.0	440.0	45.6	377.0	101.0	6.57	68.6	219	72.90	160.0	123.9	7.7
LC-1A	145.0	89.5	6.23	27.2	8.15	0.638	9.26	13.0	6.9	18.3	23.3	0.72
LC-1B	227.0	310.0	30.1	276.0	78.6	5.76	43.5	154.0	58.5	164	112.3	0.96
MC-1A	221.0	248.0	26.70	165.0	43.5	3.39	31.8	81.5	29.4	69.8	68.0	9.35
MC-1B	137.0	151.0	15.9	86.0	21.8	1.65	21.3	42.0	17	47.3	50.4	2.86
MC-2A	159.0	175.0	19.1	125.0	33.2	2.6	24.2	61.6	22.1	52.1	53.2	4.98
MC-2B	220.0	242.0	26.9	164.0	42.2	3.2	32.2	86.7	29.6	84	69.2	14.2
MC-3A	131.0	149.0	15.0	105.0	29.4	2.2	19.9	54.2	19.7	57.3	41.3	5.68
MC-3B	196.0	248.0	25.4	160.0	41.0	3.3	31.2	76.0	27.7	63.9	56.0	18.00
PC-1A	1470.0	1890.0	185.0	1190.0	281.0	25.0	263.0	549.0	225.0	297	380.7	31.1
PC-1B	448.0	517.0	46.2	285.0	72.9	5.7	71.1	130.0	54.3	124	121.2	24.5
PC-2A	106.0	118.0	10.6	58.5	12.2	1.1	10.6	24.0	8.4	12.4	19.8	1.24
PC-2B	22.0	25.0	2.7	17.7	4.7	0.4	3.2	10.0	3.4	8.89	11.6	1.03
PC-3A	33.2	36.6	4.5	22.8	5.8	0.5	5.0	11.7	4.3	11.5	11.0	1.89
PC-3B	23.4	24.4	2.7	13.4	3.5	0.3	3.1	7.2	2.7	7.29	6.9	0.60
EPA Split Samples												
D1-1A	110	91	13	67	22	16	23	46	42	55	51.3	2.29
D2-1A	400	460	92	1000	340	210	170	1000	850	570	560.0	3.03
EC-2B	10	13	1.6	14	4.3	2.8	4.2	12	11	15	16.9	5.67
EC-4A	540	490	140	1500	470	370	210	1700	1500	980	913.3	28.80
EC-4B	520	690	73	680	200	110	160	410	350	300	300	7.66
LC-1A	140	94	6.7	33	11	5.3	15	15	16	19	32.0	0.72
LC-1B	240	360	27	310	94	50	76	180	150	180	158.8	0.96
MC-3A	140	150	17	110	36	19	33	73	65	66	61.6	5.68
MC-3B	180	190	22	130	40	23	39	76	66	61	66.3	18.00
PC-1A	530	580	75	430	130	86	150	270	250	190	240.0	31.10
PC-1B	230	240	26	160	50	29	65	100	95	110	104.6	24.50
PC-2B	21	22	2.6	17.0	5.0	2.7	6.3	11.0	9.5	8.4	13.5	1.03

Notes:

HpCDD Heptachlorodibenzo-p-dioxin
HxCDD Hexachlorodibenzo-p-dioxin
PeCDD Pentachlorodibenzo-p-dioxin
OCDD Octachlorodibenzo-p-dioxin
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TEQ Toxicity Equivalence
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TEF Source: Berg et al Berg, Martin Van Den, et al. "The 2005 World Health Organization Reevaluation of Human and Mammalian Toxic Equivalency Factors for Dioxins and Dioxin-Like Compounds." Toxicological Sciences, vol. 93, no. 2, 2006, pp. 223–241., doi:10.1093/toxsci/kfl055.

Table 2b. 2018 Co-location Sampling: Total Homologue Results

Location	Total OCDF (ng/kg)	Total HpCDF (ng/kg)	Total HxCDF (ng/kg)	Total PeCDF (ng/kg)	Total TCDF (ng/kg)	Total OCDD (ng/kg)	Total HpCDD (ng/kg)	Total HxCDD (ng/kg)	Total PeCDD (ng/kg)	Total TCDD (ng/kg)	Total Furans (ng/kg)	Total Homologues (ng/kg)
D1-1A	125	243	315	284	239	4420	1620	703	101	64.0	1206	8114
D1-1B	166	341	421	367	346	4540	1830	771	100	61.6	1641	8944
D1-2A	53.5	120	156	127	108	4020	1560	658	91.2	51.2	565	6945
D1-2B	51.4	125	165	135	124	3590	1370	592	84.9	48.1	600	6285
D2-1A	190	448	1040	1210	943	4200	1640	643	101	55.6	3831	10471
D2-1B	124	328	764	956	990	3540	1380	571	83.7	45.4	3162	8782
EC-1A	90.2	198	277	235	199	4820	1640	719	102	57.1	999	8337
EC-1B	90.7	188	264	235	224	4010	1530	630	93.5	54.7	1002	7320
EC-2A	162	335	527	514	492	5110	1730	757	107	69.0	2030	9803
EC-2B	21.0	39.2	59.0	55.3	55.4	2360	644	426	65.6	34.7	230	3760
EC-3A	344	644	1080	992	750	3700	1180	515	88.9	49.8	3810	9344
EC-3B	937	1600	5420	7470	5310	6950	2600	735	124	82.4	20737	31228
EC-4A	985	1600	4870	5860	3750	6050	2190	744	128	80.2	17065	26257
EC-4B	305	696	1200	738	507	4240	1410	636	56.0	10.3	3446	9798
LC-1A	145	240	176	107	60.2	4550	1270	240	38.9	11.6	728	6839
LC-1B	227	628	876	679	548	8520	3160	636	75.4	44.4	2958	15394
MC-1A	221	435	578	457	398	5540	1780	720	122	57.4	2089	10308
MC-1B	137	287	383	305	297	5610	1950	880	124	67.3	1409	10040
MC-2A	159	312	426	326	292	4670	1600	663	91.5	54.8	1515	8594
MC-2B	220	423	567	456	423	4560	1650	673	87.9	55.9	2089	9116
MC-3A	131	250	355	308	314	2440	855	313	41.1	25.8	1358	5033
MC-3B	196	397	514	393	372	2790	916	355	56.9	28.4	1872	6018
PC-1A	1470	3670	4110	2510	1550	20000	5890	1330	145	91.3	13310	40766
PC-1B	448	1050	1250	999	864	9760	2880	899	134	76.8	4611	18361
PC-2A	106	191	168	106	78.3	1890	562	263	68.1	102	649	3534
PC-2B	22.0	42.0	56.0	42.9	43.8	2150	606	342	95.4	73.2	207	3473
PC-3A	33.2	69.5	87.1	63.8	62.6	909	307	130	16.6	12.2	316	1691
PC-3B	23.4	44.0	53.4	42.7	42.7	615	202	85.7	10.7	8.0	206	1128
EPA Split Samples												
D1-1A	110	210	320	330	290	2900	1100	620	140	64		
D2-1A	400	830	2600	3500	2300	4100	1600	720	140	84		
EC-2B	10	23	51	66	86	1100	420	370	91	50		
EC-4A	540	950	3500	5700	4200	2400	1600	600	150	110		
EC-4B	520	1200	2200	2400	2200	5400	2100	830	150	71		
LC-1A	140	250	220	140	120	4800	1300	280	56	31		
LC-1B	240	670	1000	820	720	7200	2300	610	110	53		
MC-3A	140	260	410	400	400	2000	630	310	63	33		
MC-3B	180	320	460	410	380	2000	670	350	69	36		
PC-1A	530	1300	1900	1600	1300	6900	2600	910	170	98		
PC-1B	230	530	790	750	790	4200	1400	590	120	80		
PC-2B	21	38	59	54	45	1800	500	320	88	70		

Notes:

Total homologues are reported from the laboratory report

OCDF Octachlorodibenzofuran
HpCDF Heptachlorodibenzofuran
HxCDF Hexachlorodibenzofuran
PeCDF Pentachlorodibenzofuran
TCDF Tetrachlorodibenzofuran
OCDD Octachlorodibenzo-p-dioxin
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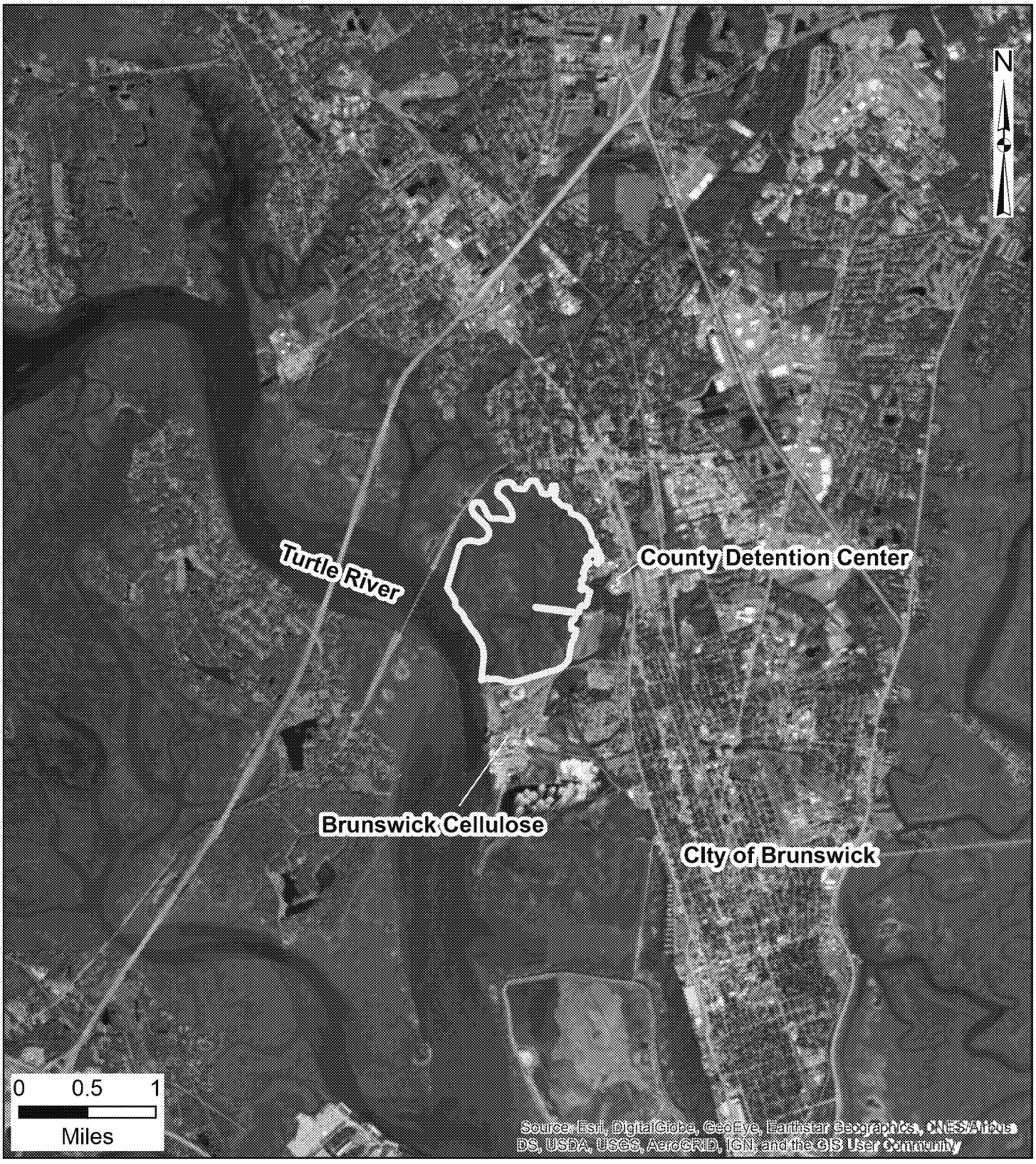
HxCDD Hexachlorodibenzo-p-dioxin
PeCDD Pentachlorodibenzo-p-dioxin
TCDD Tetrachlorodibenzo-p-dioxin

* Total homologues are reported from the laboratory report

FIGURES



OU1 (LCP Marsh)

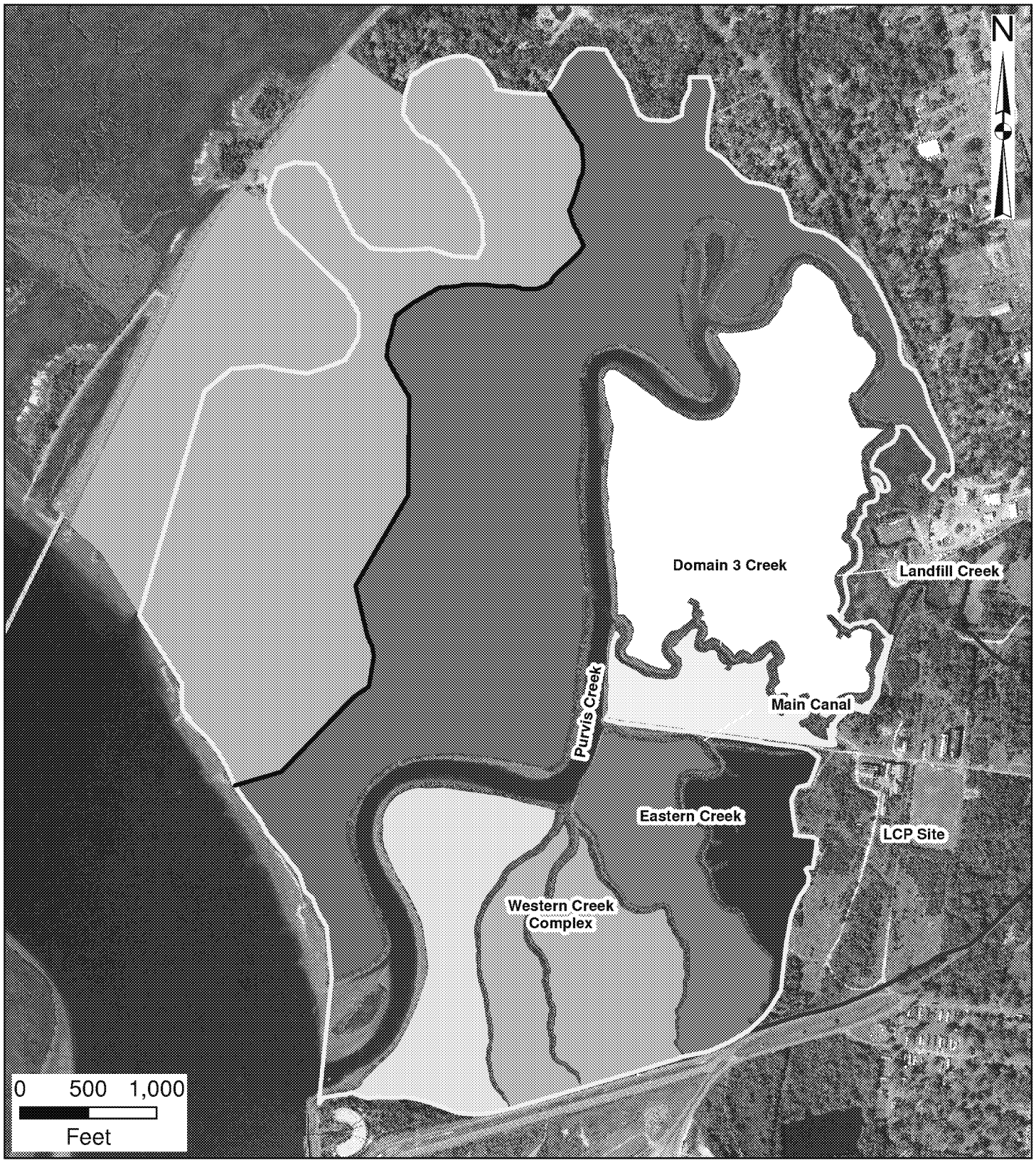
LCP Uplands

Site Location Map

LCP Chemicals Site
Brunswick, GA

Environmental Planning Specialists, Inc.

Figure No. 1



Primary Tidal Node
OU1 (LCP Marsh)
LCP Uplands

Domain Name

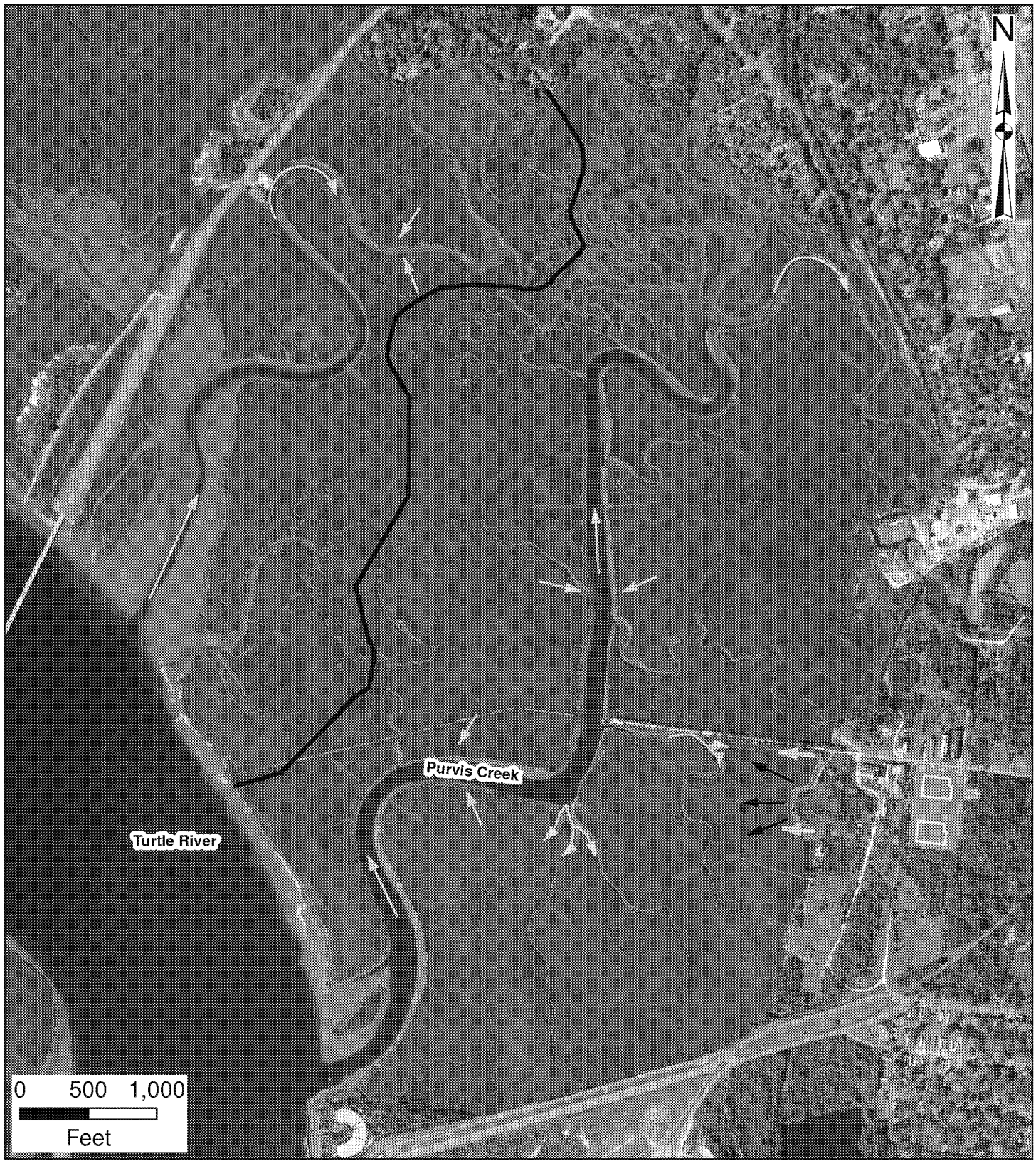
Domain 1
Domain 2a
Domain 2b
Domain 2c
Domain 2d
Domain 3a
Domain 3b
Domain 4a
Domain 4b

OU1 Features

LCP Chemicals Site
Brunswick, GA

Environmental Planning Specialists, Inc.

Figure No. 2



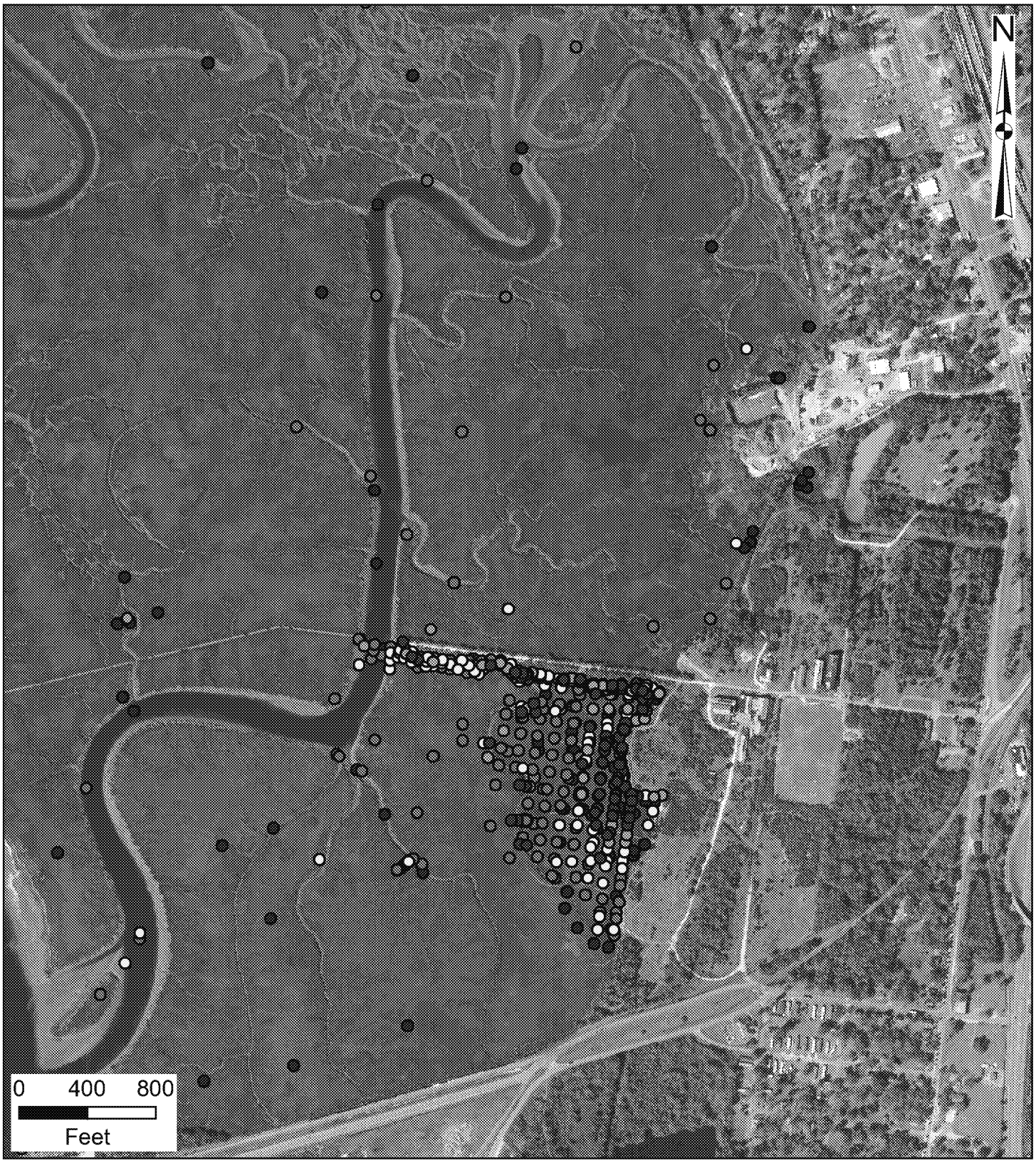
Primary Wastewater Discharge Point
Process Piping
Cell Buildings
Primary Tidal Node
Ebb tide- early stage
Ebb tide- late stage
Surface erosion and tidal mixing
Flood tide- early stage
Flood tide- late stage

OU1 Conceptual Site Model Features

LCP Chemicals Site
Brunswick, GA

Environmental Planning Specialists, Inc.

Figure No. 3



Aroclor 1268

- <1 mg/kg
- 1-10 mg/kg
- 10-50 mg/kg
- 50-100 mg/kg
- >100 mg/kg

Aroclor 1268 Condition in OU1
Prior to the 1998-99 Removal Action

LCP Chemicals Site
Brunswick, GA

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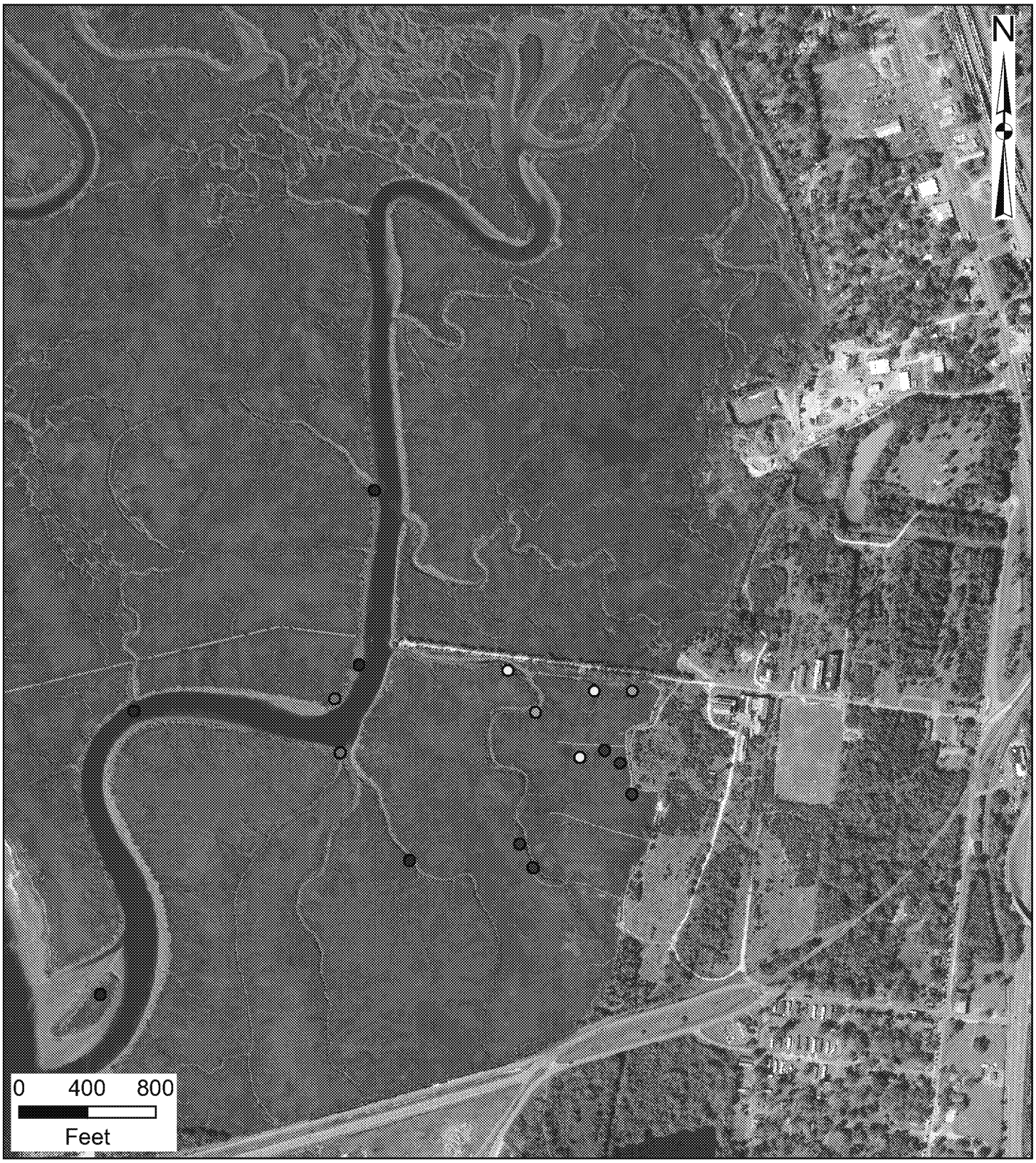
Figure No. 4



TEQ

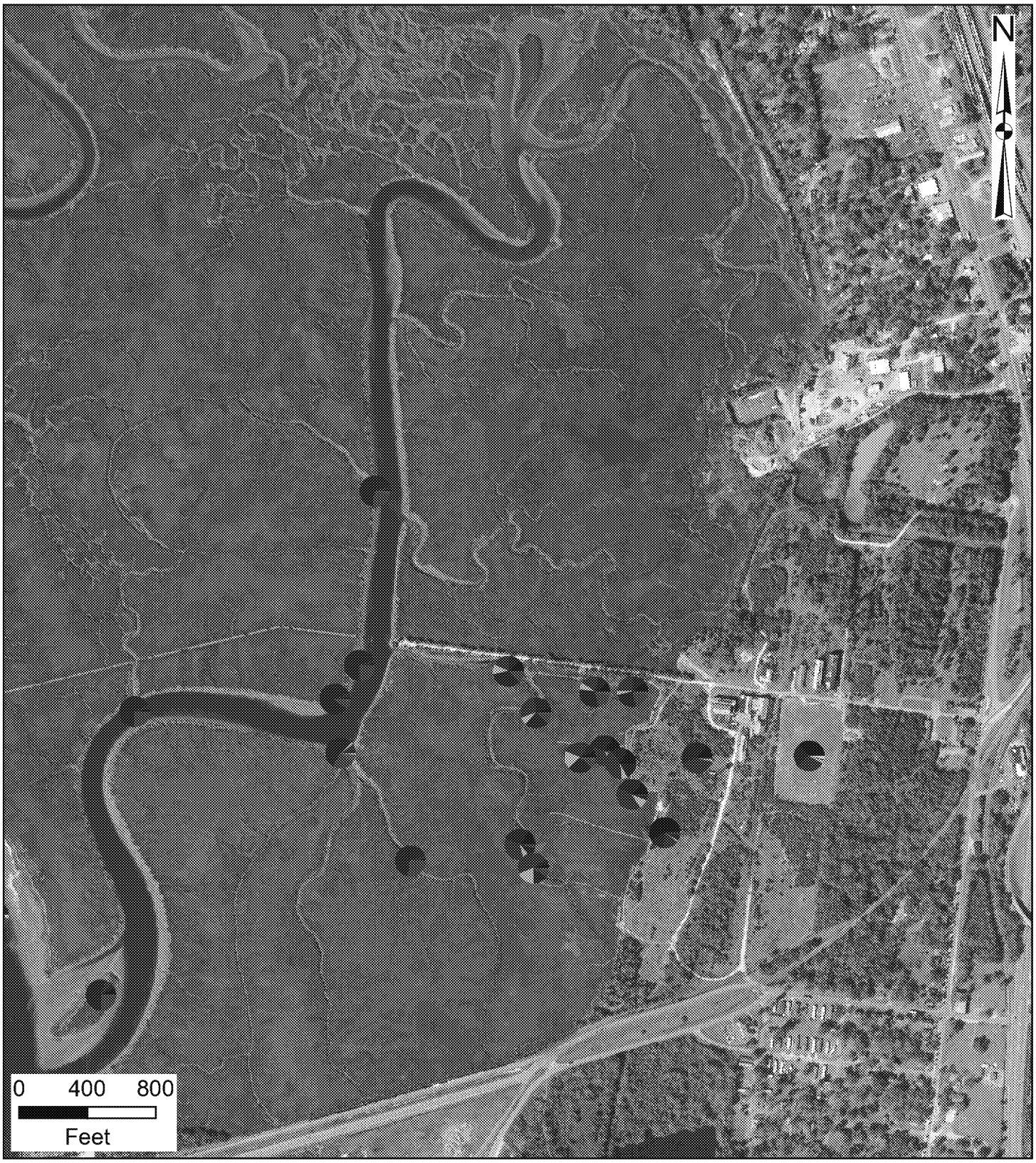
- <10 ng/kg
- 19-100 ng/kg
- 100-260 ng/kg
- 260-1000 ng/kg
- >1000 ng/kg

Dioxin TEQ Condition in OU1 Prior to the 1998-99 Removal Action

LCP Chemicals Site
Brunswick, GA

Environmental Planning Specialists, Inc.

Figure No. 5



Congener Profile

OCDF
HpCDF
HxCDF
PeCDF
TCDF
OCDD
HpCDD
HxCDD
PeCDD
TCDD

PCDD/F Congener Profile of Soil/Sediment Locations in OU1 Prior to the 1998-99 Removal Action

LCP Chemicals Site
Brunswick, GA

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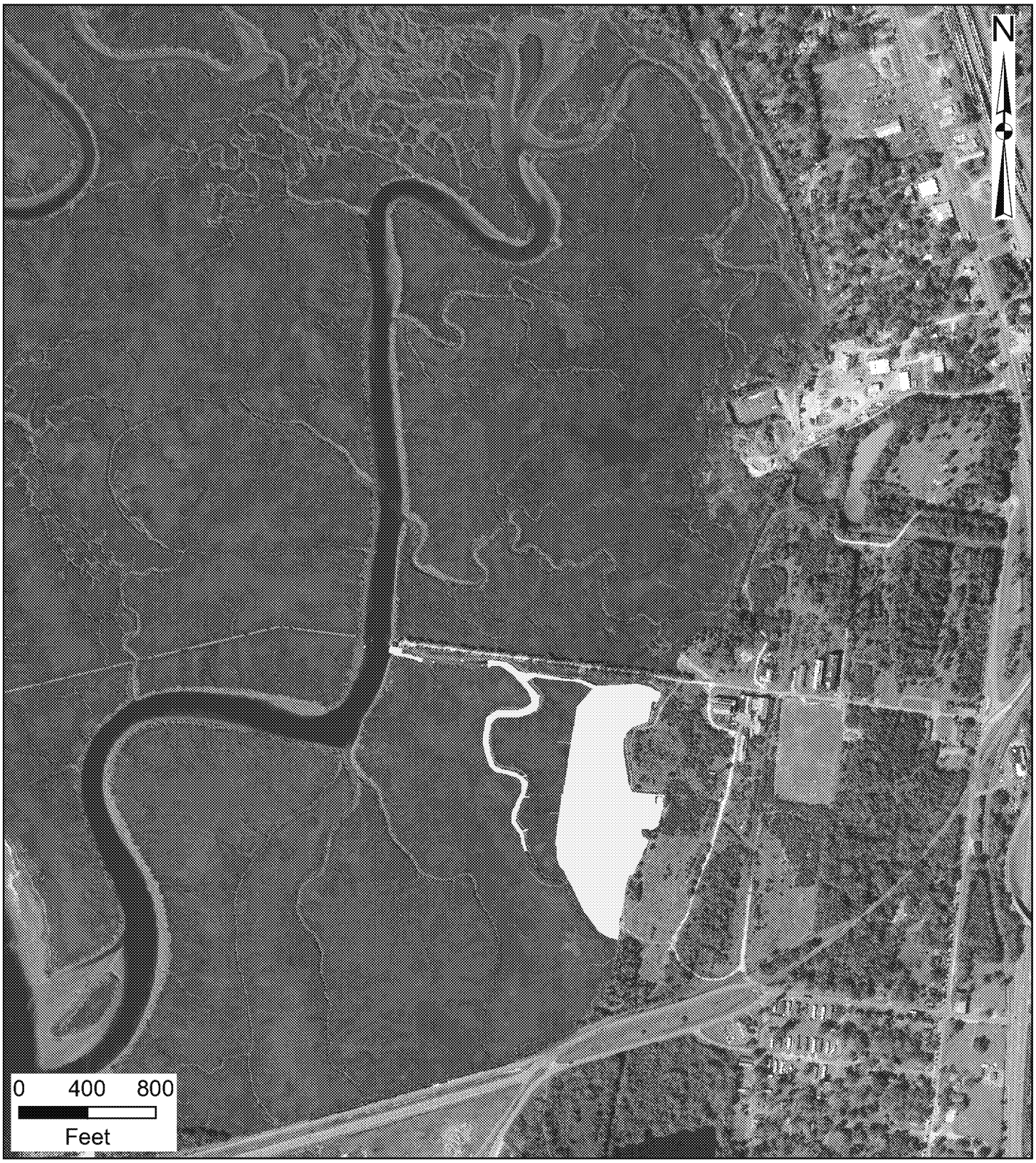
Figure No. 6



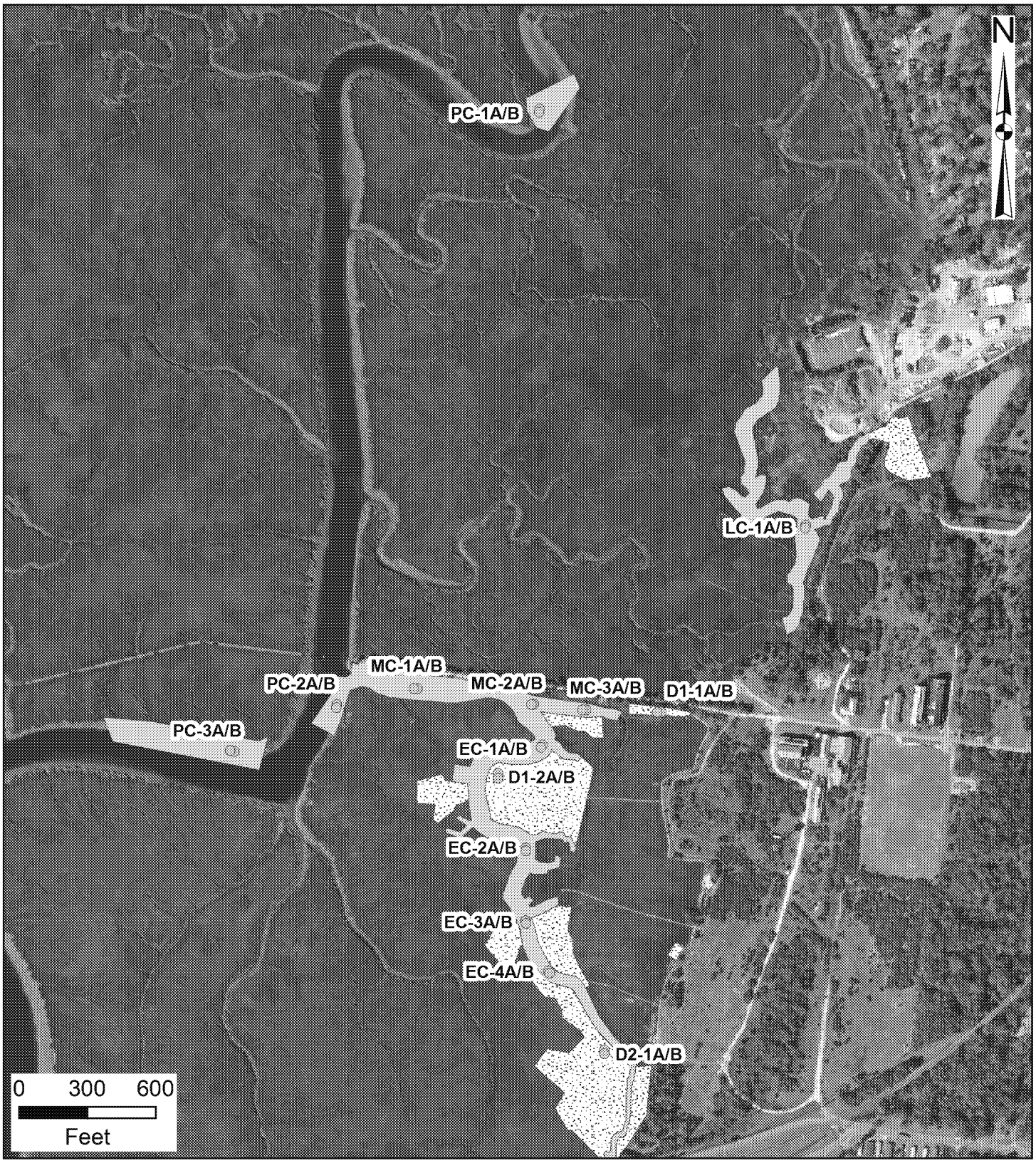
Marsh Removal Area

Marsh Removal Action Areas (1998/1999)

LCP Chemicals Site
Brunswick, GA

Environmental Planning Specialists, Inc.

Figure No. 7



Sediment Sampling Location

For each paired sample set, sample A is the northern or eastern sample location, sample B is the southern or western sample location.

OU1 Selected Remedy

Cap

Dredge

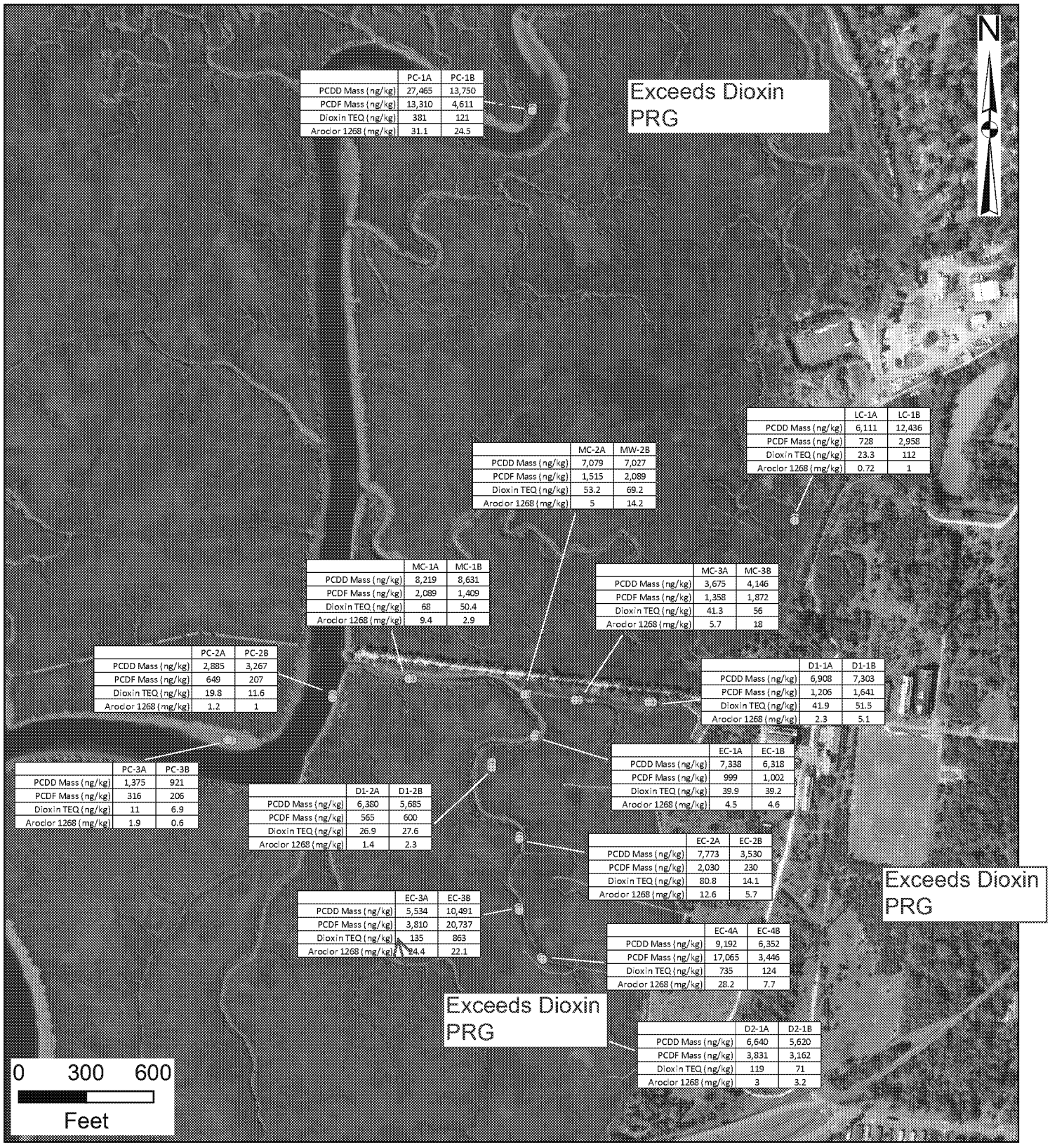
Thin Cover

Co-location Study Sampling Locations

LCP Chemicals Site
Brunswick, GA

Environmental Planning Specialists, Inc.

Figure No. 8



	PC-1A	PC-1B
PCDD Mass (ng/kg)	27,465	13,750
PCDF Mass (ng/kg)	13,310	4,611
Dioxin TEQ (ng/kg)	381	121
Aroclor 1268 (mg/kg)	31.1	24.5

	LC-1A	LC-1B
PCDD Mass (ng/kg)	6,111	12,436
PCDF Mass (ng/kg)	728	2,958
Dioxin TEQ (ng/kg)	23.3	112
Aroclor 1268 (mg/kg)	0.72	1

	MC-2A	MW-2B
PCDD Mass (ng/kg)	7,079	7,027
PCDF Mass (ng/kg)	1,515	2,089
Dioxin TEQ (ng/kg)	53.2	69.2
Aroclor 1268 (mg/kg)	5	14.2

	MC-1A	MC-1B
PCDD Mass (ng/kg)	8,219	8,631
PCDF Mass (ng/kg)	2,089	1,409
Dioxin TEQ (ng/kg)	68	50.4
Aroclor 1268 (mg/kg)	9.4	2.9

	MC-3A	MC-3B
PCDD Mass (ng/kg)	3,675	4,146
PCDF Mass (ng/kg)	1,358	1,872
Dioxin TEQ (ng/kg)	41.3	56
Aroclor 1268 (mg/kg)	5.7	18

	PC-2A	PC-2B
PCDD Mass (ng/kg)	2,885	3,267
PCDF Mass (ng/kg)	649	207
Dioxin TEQ (ng/kg)	19.8	11.6
Aroclor 1268 (mg/kg)	1.2	1

	D1-1A	D1-1B
PCDD Mass (ng/kg)	6,908	7,303
PCDF Mass (ng/kg)	1,206	1,641
Dioxin TEQ (ng/kg)	41.9	51.5
Aroclor 1268 (mg/kg)	2.3	5.1

	PC-3A	PC-3B
PCDD Mass (ng/kg)	1,375	921
PCDF Mass (ng/kg)	316	206
Dioxin TEQ (ng/kg)	11	6.9
Aroclor 1268 (mg/kg)	1.9	0.6

	D1-2A	D1-2B
PCDD Mass (ng/kg)	6,380	5,685
PCDF Mass (ng/kg)	565	600
Dioxin TEQ (ng/kg)	26.9	27.6
Aroclor 1268 (mg/kg)	1.4	2.3

	EC-1A	EC-1B
PCDD Mass (ng/kg)	7,338	6,318
PCDF Mass (ng/kg)	999	1,002
Dioxin TEQ (ng/kg)	39.9	39.2
Aroclor 1268 (mg/kg)	4.5	4.6

	EC-2A	EC-2B
PCDD Mass (ng/kg)	7,773	3,530
PCDF Mass (ng/kg)	2,030	230
Dioxin TEQ (ng/kg)	80.8	14.1
Aroclor 1268 (mg/kg)	12.6	5.7

	EC-3A	EC-3B
PCDD Mass (ng/kg)	5,534	10,491
PCDF Mass (ng/kg)	3,810	20,737
Dioxin TEQ (ng/kg)	135	863
Aroclor 1268 (mg/kg)	24.4	22.1

	EC-4A	EC-4B
PCDD Mass (ng/kg)	9,192	6,352
PCDF Mass (ng/kg)	17,065	3,446
Dioxin TEQ (ng/kg)	735	124
Aroclor 1268 (mg/kg)	28.2	7.7

	D2-1A	D2-1B
PCDD Mass (ng/kg)	6,640	5,620
PCDF Mass (ng/kg)	3,831	3,162
Dioxin TEQ (ng/kg)	119	71
Aroclor 1268 (mg/kg)	3	3.2

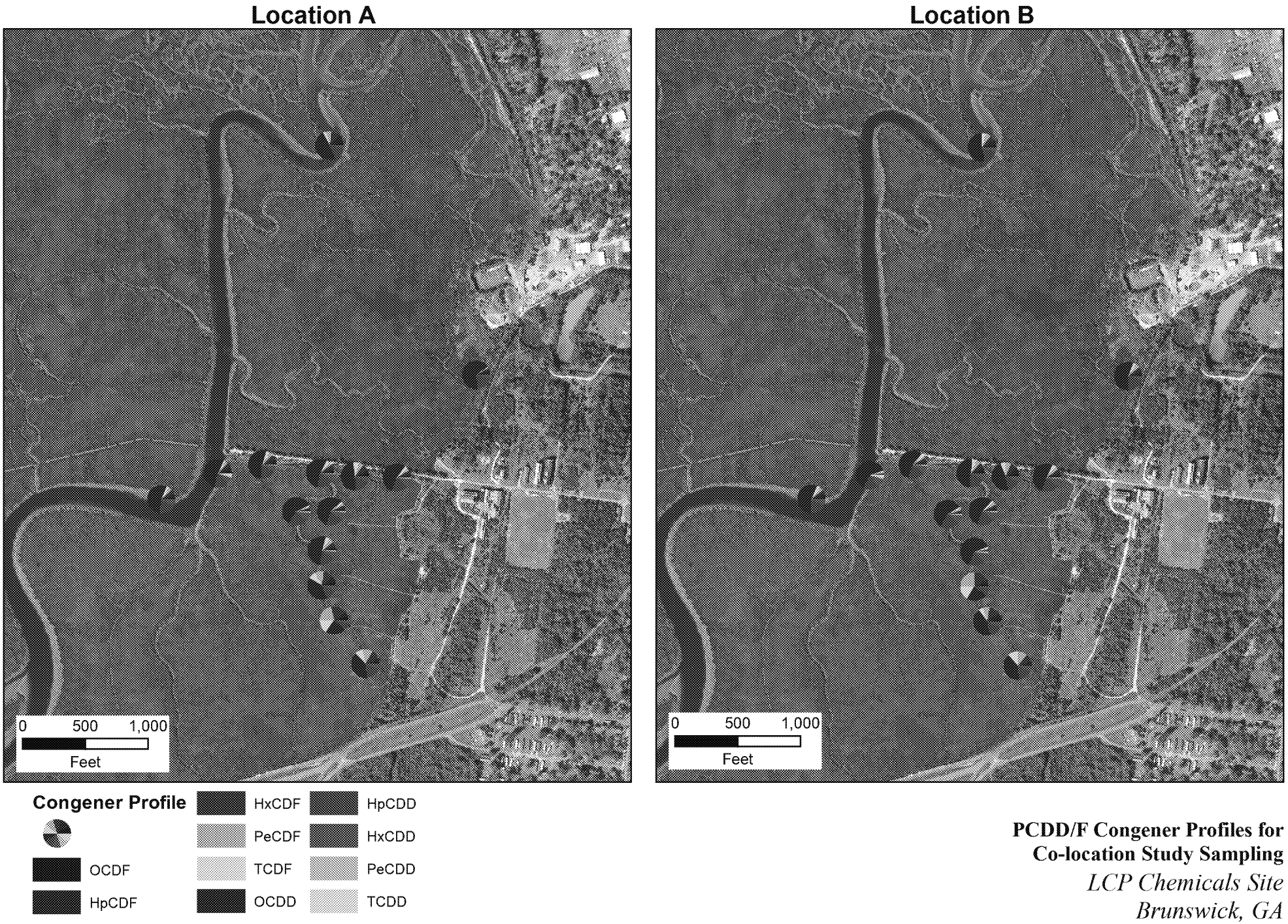
Sediment Sampling Location

Co-location Study Sampling Results

LCP Chemicals Site
Brunswick, GA

Environmental Planning Specialists, Inc.

Figure No. 9



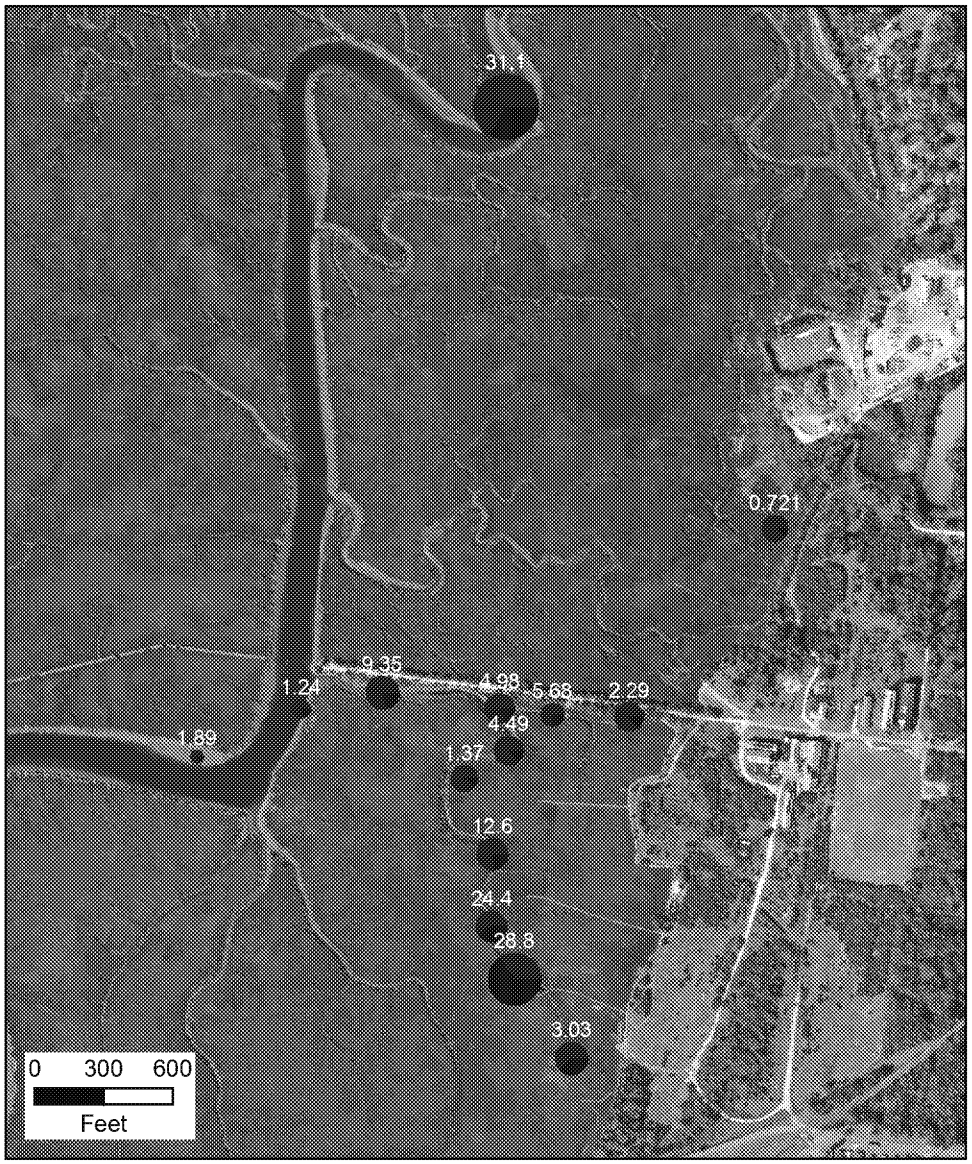
PCDD/F Congener Profiles for Co-location Study Sampling

LCP Chemicals Site
Brunswick, GA

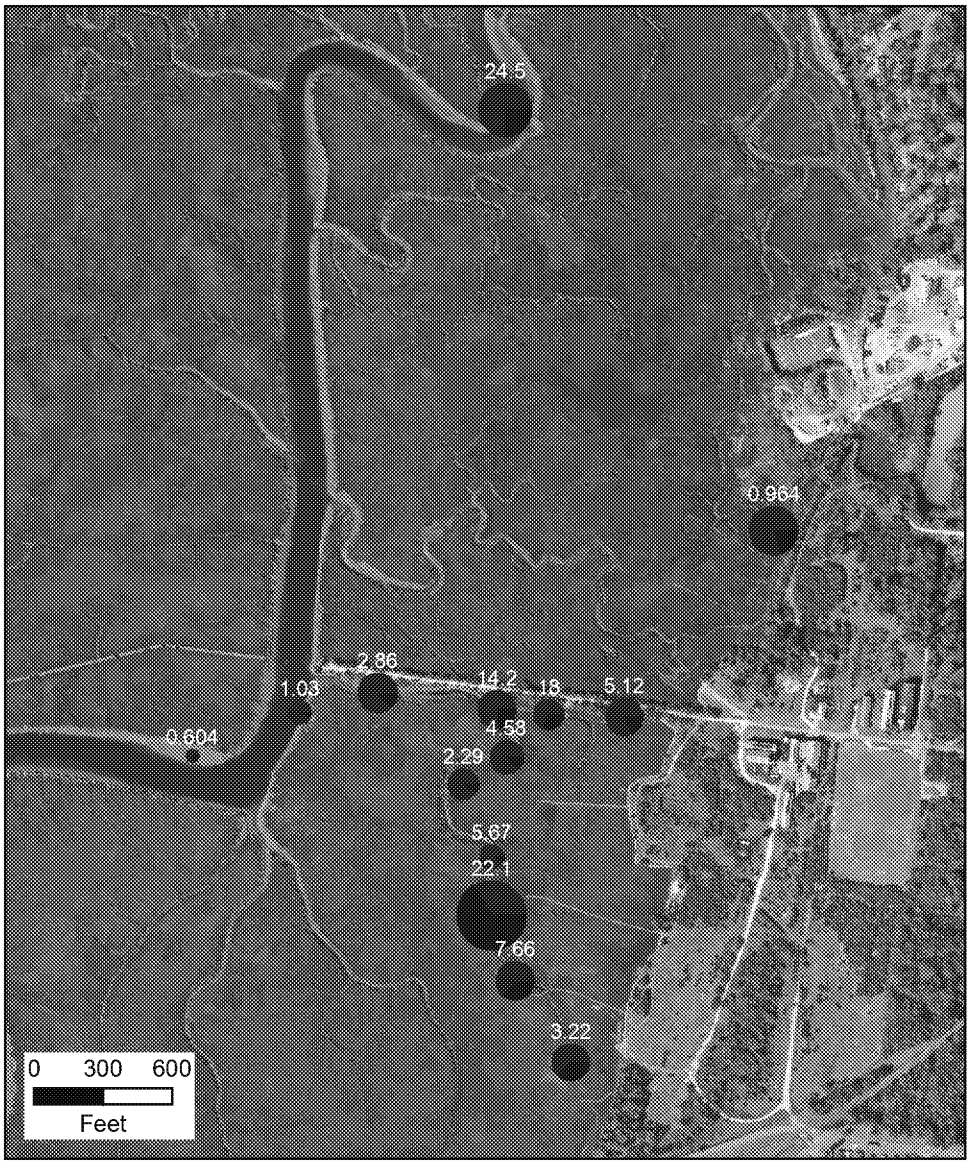
Environmental Planning Specialists, Inc.

Figure No. 10

Location A



Location B



PCDD/F Congener Profile

Dioxin Portion of Total PCDD/F

Furan Portion of Total PCDD/F

Notes:
1. The figure depicts both the total PCDD/F mass and Aroclor 1268 mass (concentration).
2. Total PCDD/F relative mass concentration is depicted by the proportional size of the circle.
3. Aroclor 1268 concentration is depicted by the value posted at each sampling location.
4. Aroclor 1268 results in mg/kg.

2018 Co-location Study Results
Total PCDD/F Mass Concentration and Corresponding Aroclor 1268 Concentration

LCP Chemicals Site
Brunswick, GA

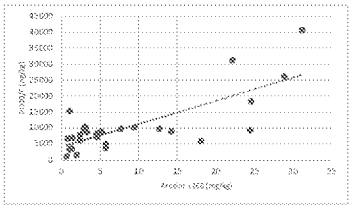
Environmental Planning Specialists, Inc.

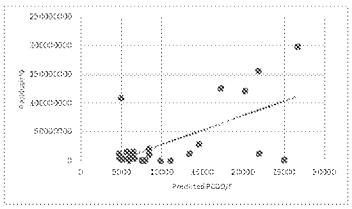
Figure No. 11

APPENDIX B
Testing of Linear Regression Assumptions for Co-location Cases 1-3

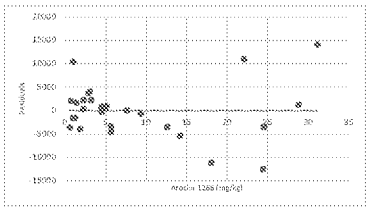
Case 1a: Furan Congener Concentration and Aroclor 1268 (Co-location Study Data)

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)	Pred PCDD/F (ng/kg)	Pred PCDD/F^2	Residual PCDD/F	Residual^2
D1-1A	8114.0	2.29	5911.96	34951311.31	2202.04	4848965.16
D1-1B	8943.5	5.12	7951.19	63221397.64	992.31	984682.23
D1-2A	6944.9	1.37	5249.04	27552369.75	1695.86	2875957.67
D1-2B	6285.4	2.29	5911.96	34951311.31	373.44	139454.89
D2-1A	10470.6	3.03	6445.19	41540452.57	4025.41	16203939.14
D2-1B	8782.1	3.22	6582.10	43324006.55	2200.00	4840011.32
EC-1A	8337.3	4.49	7497.23	56208407.96	840.07	705723.17
EC-1B	7319.9	4.58	7562.08	57185029.19	-242.18	58650.36
EC-2A	9803.0	12.6	13341.08	177984511.38	-3538.08	12518035.50
EC-2B	3760.2	5.67	8347.50	69680827.40	-4587.30	21043360.39
EC-3A	9343.7	24.4	21843.86	477154191.77	-12500.16	156253984.04
EC-3B	31228.4	22.1	20186.54	407496343.07	11041.86	121922701.85
EC-4A	26257.2	28.8	25014.39	625719502.90	1242.81	1544586.84
EC-4B	9798.3	7.66	9781.45	95676704.54	16.85	284.03
LC-1A	6838.7	0.721	4781.38	22861618.21	2057.32	4232555.47
LC-1B	15393.8	0.964	4956.48	24566713.75	10437.32	108937607.18
MC-1A	10308.4	9.35	10999.22	120982783.04	-690.82	477228.66
MC-1B	10040.3	2.86	6322.69	39976417.81	3717.61	13820618.83
MC-2A	8594.3	4.98	7850.31	61627336.50	743.99	553524.02
MC-2B	9115.8	14.2	14494.00	210076103.82	-5378.20	28925060.40
MC-3A	5032.9	5.68	8354.71	69801179.25	-3321.81	11034421.70
MC-3B	6018.3	18	17232.18	296948178.06	-11213.88	125751202.60
PC-1A	40766.3	31.1	26671.71	711379934.02	14094.59	198657562.55
PC-1B	18360.8	24.5	21915.92	480307408.42	-3555.12	12638855.34
PC-2A	3534.4	1.24	5155.36	26577741.65	-1620.96	2627512.87
PC-2B	3473.3	1.03	5004.04	25040415.23	-1530.74	2343164.61
PC-3A	1691.0	1.89	5623.73	31626380.94	-3932.73	15466394.50
PC-3B	1127.6	0.604	4697.08	22062516.13	-3569.51	12741367.90





Test for Zero Conditional Mean of Errors



No discernable relationship between residuals and independent variable
$Cov(\hat{u}, x_i) = 0$

Tests for Homoscedasticity

BREUSCH-PAGAN SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.620776693
R Square	0.385363703
Adjusted R Square	0.361723845
Standard Error	43838768.96
Observations	28

$$\hat{u}^2 = d_0 + x d_1$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p<0.05
Status: Heteroscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	3.13287E+16	3.13287E+16	16.30143927	0.000423921
Residual	26	4.99678E+16	1.92184E+15		
Total	27	8.12965E+16			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-229567.4794	11420019.9	-0.020102196	0.984115326	-23703754.57	23244619.61	-23703754.57	23244619.61
Ar1268 (mg/kg)	3630705.783	899245.1036	4.037504089	0.000423921	1782281	5479130.566	1782281	5479130.566

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.643059799
R Square	0.413525905
Adjusted R Square	0.366607978
Standard Error	43670718.25
Observations	28

$$\hat{u}^2 = d_0 + \hat{Y} \times d_1 + \hat{Y}^2 \times d_2$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p<0.05
Status: Heteroscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	2	3.36182E+16	1.68091E+16	8.813814385	0.001267974
Residual	25	4.76783E+16	1.90713E+15		
Total	27	8.12965E+16			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	17870835.75	39306881.44	0.454649036	0.653285044	-63083201.98	98824873.47	-63083201.98	98824873.47
Pred PCDD/F (ng/kg)	-2588.756137	7071.534772	-0.366081229	0.717394202	-17152.85463	11975.34235	-17152.85463	11975.34235
Pred PCDD/F^2	0.2633361	0.240343015	1.09566779	0.283667507	-0.231659605	0.758331804	-0.231659605	0.758331804

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight	Weight * X	Weight * X^2
D1-1A	8114.0	2.29	5911.96	2202.037	2202.04	2382.20015	1.76215E-07	4.03533E-07	9.2409E-07
D1-1B	8943.5	5.12	7951.19	992.312	992.31	3081.969977	1.05279E-07	5.3903E-07	2.75983E-06
D1-2A	6944.9	1.37	5249.04	1695.865	1695.86	2154.713139	2.15388E-07	2.95081E-07	4.04261E-07
D1-2B	6285.4	2.29	5911.96	373.437	373.44	2382.20015	1.76215E-07	4.03533E-07	9.2409E-07
D2-1A	10470.6	3.03	6445.19	4025.412	4025.41	2565.178832	1.51972E-07	4.60476E-07	1.39524E-06
D2-1B	8782.1	3.22	6582.10	2200.003	2200.00	2612.159846	1.46555E-07	4.71907E-07	1.51954E-06
EC-1A	8337.3	4.49	7497.23	840.073	840.07	2926.190828	1.16787E-07	5.24374E-07	2.35444E-06
EC-1B	7319.9	4.58	7562.08	-242.178	242.18	2948.444992	1.15031E-07	5.26841E-07	2.41293E-06
EC-2A	9803.0	12.6	13341.08	-3538.084	3538.08	4931.538284	4.11183E-08	5.18091E-07	6.52794E-06
EC-2B	3760.2	5.67	8347.50	-4587.304	4587.30	3217.967647	9.65688E-08	5.47545E-07	3.10458E-06
EC-3A	9343.7	24.4	21843.86	-12500.159	12500.16	7849.306469	1.62307E-08	3.96029E-07	9.66311E-06
EC-3B	31228.4	22.1	20186.54	11041.861	11041.86	7280.588942	1.88654E-08	4.16926E-07	9.21407E-06
EC-4A	26257.2	28.8	25014.39	1242.814	1242.81	8937.287826	1.25195E-08	3.60563E-07	1.03842E-05
EC-4B	9798.3	7.66	9781.45	16.853	16.85	3710.031942	7.26515E-08	5.56511E-07	4.26287E-06
LC-1A	6838.7	0.721	4781.38	2057.318	2057.32	1994.235888	2.51447E-07	1.81293E-07	1.30713E-07
LC-1B	15393.8	0.964	4956.48	10437.318	10437.32	2054.322132	2.36953E-07	2.28423E-07	2.202E-07
MC-1A	10308.4	9.35	10999.22	-690.817	690.82	4127.915691	5.86865E-08	5.48719E-07	5.13052E-06
MC-1B	10040.3	2.86	6322.69	3717.609	3717.61	2523.143189	1.57078E-07	4.49244E-07	1.28484E-06
MC-2A	8594.3	4.98	7850.31	743.992	743.99	3047.352388	1.07685E-07	5.36271E-07	2.67063E-06
MC-2B	9115.8	14.2	14494.00	-5378.202	5378.20	5327.167869	3.52377E-08	5.00375E-07	7.10532E-06
MC-3A	5032.9	5.68	8354.71	-3321.810	3321.81	3220.440332	9.64205E-08	5.47669E-07	3.11076E-06
MC-3B	6018.3	18	17232.18	-11213.884	11213.88	6266.788132	2.5463E-08	4.58334E-07	8.25002E-06
PC-1A	40766.3	31.1	26671.71	14094.593	14094.59	9506.005354	1.10663E-08	3.44163E-07	1.07035E-05
PC-1B	18360.8	24.5	21915.92	-3555.117	3555.12	7874.033318	1.61289E-08	3.95159E-07	9.68139E-06
PC-2A	3534.4	1.24	5155.36	-1620.960	1620.96	2122.568235	2.21961E-07	2.75232E-07	3.41287E-07
PC-2B	3473.3	1.03	5004.04	-1530.740	1530.74	2070.641852	2.33233E-07	2.4023E-07	2.47437E-07
PC-3A	1691.0	1.89	5623.73	-3932.734	3932.73	2283.292754	1.91812E-07	3.62526E-07	6.85173E-07
PC-3B	1127.6	0.604	4697.08	-3569.505	3569.51	1965.305475	2.58905E-07	1.56378E-07	9.44526E-08
						SUM	3.36348E-06	1.16445E-05	0.000105507

OLS Error Variance **15339**

$$Var = \frac{\sum w_i}{\left((\sum w_i)(\sum w_i x_i^2) - (\sum w_i x_i)^2\right)}$$

Case 1a: Furan Congener Concentration and Aroclor 1268 (Co-location Study Data)

Location	Y-PCDD/F [ng/kg]	X-Ar1268 [mg/kg]
D1-1A	8114.0	2.29
D1-1B	8943.5	5.12
D1-2A	6944.9	1.37
D1-2B	6285.4	2.29
D2-1A	10470.6	3.03
D2-1B	8782.1	3.22
EC-1A	8337.3	4.49
EC-1B	7319.9	4.58
EC-2A	9803.0	12.6
EC-2B	3760.2	5.67
EC-3A	9343.7	24.4
EC-3B	31228.4	22.1
EC-4A	26257.2	28.8
EC-4B	9798.3	7.66
LC-1A	6838.7	0.721
LC-1B	15393.8	0.964
MC-1A	10308.4	9.35
MC-1B	10040.3	2.86
MC-2A	8594.3	4.98
MC-2B	9115.8	14.2
MC-3A	5032.9	5.68
MC-3B	6018.3	18
PC-1A	40766.3	31.1
PC-1B	18360.8	24.5
PC-2A	3534.4	1.24
PC-2B	3473.3	1.03
PC-3A	1691.0	1.89
PC-3B	1127.6	0.604

Weighted Least Squares performed with "Real Stats" Add-In

$$Pred\ Y_i' = Abs(Res)\alpha + \partial_1$$

$$W_i = \frac{1}{Pred\ Y_i'^2}$$

WLS solution is asymptotic at Iteration #4.

Iteration #1

Location	Y-PCDD/F [ng/kg]	X-Ar1268 [mg/kg]	Pred Y	Residual	ABS(Res)	Pred Y'	Weight
D1-1A	8114.0	2.29	5.91E+03	2.20E+03	2.20E+03	2.38E+03	1.76E-07
D1-1B	8943.5	5.12	7.95E+03	9.92E+02	9.92E+02	3.08E+03	1.05E-07
D1-2A	6944.9	1.37	5.25E+03	1.70E+03	1.70E+03	2.15E+03	2.15E-07
D1-2B	6285.4	2.29	5.91E+03	3.73E+02	3.73E+02	2.38E+03	1.76E-07
D2-1A	10470.6	3.03	6.45E+03	4.03E+03	4.03E+03	2.57E+03	1.52E-07
D2-1B	8782.1	3.22	6.58E+03	2.20E+03	2.20E+03	2.61E+03	1.47E-07
EC-1A	8337.3	4.49	7.50E+03	8.40E+02	8.40E+02	2.93E+03	1.17E-07
EC-1B	7319.9	4.58	7.56E+03	-2.42E+02	2.42E+02	2.95E+03	1.15E-07
EC-2A	9803.0	12.6	1.33E+04	-3.54E+03	3.54E+03	4.93E+03	4.11E-08
EC-2B	3760.2	5.67	8.35E+03	-4.59E+03	4.59E+03	3.22E+03	9.66E-08
EC-3A	9343.7	24.4	2.18E+04	-1.25E+04	1.25E+04	7.85E+03	1.62E-08
EC-3B	31228.4	22.1	2.02E+04	1.10E+04	1.10E+04	7.28E+03	1.89E-08
EC-4A	26257.2	28.8	2.50E+04	1.24E+03	1.24E+03	8.94E+03	1.25E-08
EC-4B	9798.3	7.66	9.78E+03	1.69E+01	1.69E+01	3.71E+03	7.27E-08
LC-1A	6838.7	0.721	4.78E+03	2.06E+03	2.06E+03	1.89E+03	2.51E-07
LC-1B	15393.8	0.964	4.96E+03	1.04E+04	1.04E+04	2.05E+03	2.37E-07
MC-1A	10308.4	9.35	1.10E+04	-6.91E+02	6.91E+02	4.13E+03	5.87E-08
MC-1B	10040.3	2.86	6.32E+03	3.72E+03	3.72E+03	2.52E+03	1.57E-07
MC-2A	8594.3	4.98	7.85E+03	7.44E+02	7.44E+02	3.05E+03	1.08E-07
MC-2B	9115.8	14.2	1.45E+04	-5.38E+03	5.38E+03	5.33E+03	3.52E-08
MC-3A	5032.9	5.68	8.35E+03	-3.32E+03	3.32E+03	3.22E+03	9.64E-08
MC-3B	6018.3	18	1.72E+04	-1.12E+04	1.12E+04	6.27E+03	2.55E-08
PC-1A	40766.3	31.1	2.67E+04	1.41E+04	1.41E+04	9.51E+03	1.11E-08
PC-1B	18360.8	24.5	2.19E+04	-3.56E+03	3.56E+03	7.87E+03	1.61E-08
PC-2A	3534.4	1.24	5.16E+03	-1.62E+03	1.62E+03	2.12E+03	2.22E-07
PC-2B	3473.3	1.03	5.00E+03	-1.53E+03	1.53E+03	2.07E+03	2.33E-07
PC-3A	1691.0	1.89	5.62E+03	-3.93E+03	3.93E+03	2.28E+03	1.92E-07
PC-3B	1127.6	0.604	4.70E+03	-3.57E+03	3.57E+03	1.97E+03	2.59E-07

OVERALL FIT

Multiple R	0.528988267	AIC	20.33056889
R Square	0.279828586	AICc	20.81056889
Adjusted R Square	0.253155571	BSC	21.6627734
Standard Error	1.43962919		
Observations	28		

ANOVA (Alpha 0.05)

	df	SS	MS	F	p-value	sig
Regression	1	20.93778981	20.93778981	10.10251603	0.003800262	yes
Residual	26	53.88583732	2.072532205			
Total	27	74.82362713				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	5354.574519	998.6064587	5.362046752	1.29581E-05	3301.905545	7407.239452	
X-Ar1268 (mg/kg)	566.7111097	178.2981974	3.178445536	0.003800262	200.213916	933.2083033	1

Iteration #2

Location	Y-PCDD/F [ng/kg]	X-Ar1268 [mg/kg]	Pred Y2	Residual	ABS(Res)	Pred Y2'	Weight
D1-1A	8114.0	2.29	6.65E+03	1.46E+03	1.46E+03	2.09E+03	2.28E-07
D1-1B	8943.5	5.12	8.26E+03	6.87E+02	6.87E+02	2.89E+03	1.20E-07
D1-2A	6944.9	1.37	6.13E+03	8.14E+02	8.14E+02	1.83E+03	2.98E-07
D1-2B	6285.4	2.29	6.65E+03	-3.67E+02	3.67E+02	2.09E+03	2.28E-07
D2-1A	10470.6	3.03	7.07E+03	3.40E+03	3.40E+03	2.30E+03	1.89E-07
D2-1B	8782.1	3.22	7.18E+03	1.60E+03	1.60E+03	2.35E+03	1.80E-07
EC-1A	8337.3	4.49	7.90E+03	4.38E+02	4.38E+02	2.71E+03	1.36E-07
EC-1B	7319.9	4.58	7.95E+03	-6.30E+02	6.30E+02	2.74E+03	1.33E-07
EC-2A	9803.0	12.6	1.25E+04	-2.69E+03	2.69E+03	5.00E+03	4.00E-08
EC-2B	3760.2	5.67	8.57E+03	-4.81E+03	4.81E+03	3.04E+03	1.08E-07
EC-3A	9343.7	24.4	1.92E+04	-9.84E+03	9.84E+03	8.32E+03	1.44E-08
EC-3B	31228.4	22.1	1.79E+04	1.33E+04	1.33E+04	7.68E+03	1.70E-08
EC-4A	26257.2	28.8	2.17E+04	4.58E+03	4.58E+03	9.56E+03	1.09E-08
EC-4B	9798.3	7.66	9.70E+03	1.03E+02	1.03E+02	3.61E+03	7.69E-08
LC-1A	6838.7	0.721	5.76E+03	1.08E+03	1.08E+03	1.65E+03	3.67E-07
LC-1B	15393.8	0.964	5.90E+03	9.49E+03	9.49E+03	1.72E+03	3.39E-07
MC-1A	10308.4	9.35	1.07E+04	-3.45E+02	3.45E+02	4.08E+03	6.00E-08
MC-1B	10040.3	2.86	6.98E+03	3.06E+03	3.06E+03	2.25E+03	1.97E-07
MC-2A	8594.3	4.98	8.18E+03	4.18E+02	4.18E+02	2.85E+03	1.23E-07
MC-2B	9115.8	14.2	1.34E+04	-4.29E+03	4.29E+03	5.45E+03	3.37E-08
MC-3A	5032.9	5.68	8.57E+03	-3.54E+03	3.54E+03	3.05E+03	1.08E-07
MC-3B	6018.3	18	1.56E+04	-9.54E+03	9.54E+03	6.52E+03	2.35E-08
PC-1A	40766.3	31.1	2.30E+04	1.78E+04	1.78E+04	1.02E+04	9.59E-09
PC-1B	18360.8	24.5	1.92E+04	-8.78E+02	8.78E+02	8.35E+03	1.43E-08
PC-2A	3534.4	1.24	6.06E+03	-2.52E+03	2.52E+03	1.80E+03	3.10E-07
PC-2B	3473.3	1.03	5.94E+03	-2.46E+03	2.46E+03	1.74E+03	3.31E-07
PC-3A	1691.0	1.89	6.43E+03	-4.73E+03	4.73E+03	1.98E+03	2.55E-07
PC-3B	1127.6	0.604	5.70E+03	-4.57E+03	4.57E+03	1.62E+03	3.82E-07

OVERALL FIT

Multiple R	0.472732618	AIC	27.08475404
R Square	0.223476128	AICc	27.56475404
Adjusted R Square	0.194715985	BSC	28.41695855
Standard Error	1.624168549		
Observations	28		

ANOVA (Alpha 0.05)

	df	SS	MS	F	p-value	sig
Regression	1	19.73839645	19.7384	7.482550818	0.011073	yes
Residual	26	68.58601034	2.637923			
Total	27	88.3244068				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	5409.216818	993.5595367	5.444281	1.04447E-05	3366.926	7451.508	
X-Ar1268 (mg/kg)	555.9106008	203.2263973	2.735425	0.011073042	138.1728	973.6484	1

Iteration #3

Location	Y-PCDD/F [ng/kg]	X-Ar1268 [mg/kg]	Pred Y3	Residual	ABS(Res)	Pred Y3'	Weight
D1-1A	8114.0	2.29	6.68E+03	1.43E+03	1.43E+03	2.08E+03	2.32E-07
D1-1B	8943.5	5.12	8.26E+03	6.88E+02	6.88E+02	2.88E+03	1.21E-07
D1-2A	6944.9	1.37	6.17E+03	7.74E+02	7.74E+02	1.81E+03	3.04E-07
D1-2B	6285.4	2.29	6.68E+03	-3.97E+02	3.97E+02	2.08E+03	2.32E-07
D2-1A	10470.6	3.03	7.09E+03	3.38E+03	3.38E+03	2.29E+03	1.91E-07
D2-1B	8782.1	3.22	7.20E+03	1.58E+03	1.58E+03	2.34E+03	1.83E-07
EC-1A	8337.3	4.49	7.91E+03	4.32E+02	4.32E+02	2.70E+03	1.37E-07
EC-1B	7319.9	4.58	7.96E+03	-6.35E+02	6.35E+02	2.73E+03	1.35E-07
EC-2A	9803.0	12.6	1.24E+04	-2.61E+03	2.61E+03	5.00E+03	3.99E-08
EC-2B	3760.2	5.67	8.56E+03	-4.80E+03	4.80E+03	3.04E+03	1.09E-07
EC-3A	9343.7	24.4	1.90E+04	-9.63E+03	9.63E+03	8.36E+03	1.43E-08
EC-3B	31228.4	22.1	1.77E+04	1.35E+04	1.35E+04	7.70E+03	1.69E-08
EC-4A	26257.2	28.8	2.14E+04	4.84E+03	4.84E+03	9.61E+03	1.08E-08
EC-4B	9798.3	7.66	9.67E+03	1.31E+02	1.31E+02	3.60E+03	7.71E-08
LC-1A	6838.7	0.721	5.81E+03	1.03E+03	1.03E+03	1.63E+03	3.77E-07
LC-1B	15393.8	0.964	5.95E+03	9.45E+03	9.45E+03	1.70E+03	3.47E-07
MC-1A	10308.4	9.35	1.06E+04	-2.99E+02	2.99E+02	4.08E+03	6.01E-08
MC-1B	10040.3	2.86	7.00E+03	3.04E+03	3.04E+03	2.24E+03	2.00E-07
MC-2A	8594.3	4.98	8.18E+03	4.17E+02	4.17E+02	2.84E+03	1.24E-07
MC-2B	9115.8	14.2	1.33E+04	-4.19E+03	4.19E+03	5.46E+03	3.36E-08
MC-3A	5032.9	5.68	8.57E+03	-3.53E+03	3.53E+03	3.04E+03	1.08E-07
MC-3B	6018.3	18	1.54E+04	-9.40E+03	9.40E+03	6.54E+03	2.34E-08
PC-1A	40766.3	31.1	2.27E+04	1.81E+04	1.81E+04	1.03E+04	9.50E-09
PC-1B	18360.8	24.5	1.90E+04	-6.68E+02	6.68E+02	8.38E+03	1.42E-08
PC-2A	3534.4	1.24	6.10E+03	-2.56E+03	2.56E+03	1.78E+03	3.17E-07
PC-2B	3473.3	1.03	5.98E+03	-2.51E+03	2.51E+03	1.72E+03	3.39E-07
PC-3A	1691.0	1.89	6.46E+03	-4.77E+03	4.77E+03	1.96E+03	2.60E-07
PC-3B	1127.6	0.604	5.74E+03	-4.62E+03	4.62E+03	1.60E+03	3.92E-07

OVERALL FIT

Multiple R	0.469087363	AIC	27.5567546
R Square	0.220042954	AICc	28.0367546
Adjusted R Square	0.191155656	BSC	28.88895511
Standard Error	1.637915839		
Observations	28		

ANOVA (Alpha 0.05)

	df	SS	MS	F	p-value	sig
Regression	1	19.67855903	19.67855903	7.335169068	0.011798134	yes
Residual	26	69.75197572	2.682768297			
Total	27	89.43053475				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	5411.87551	993.716569	5.445864412	1.04607E-05	3369.061849	7454.289171	
X-Ar1268 (mg/kg)	555.4005044	205.0695629	2.708351725	0.011798134	133.873981	976.9270279	1

Iteration #4

Location	Y-PCDD/F [ng/kg]	X-Ar1268 [mg/kg]	Pred Y4	Residual	ABS(Res)	Pred Y4'	Weight
D1-1A	8114.0	2.29	6.68E+03	1.43E+03	1.43E+03	2.07E+03	2.32E-07
D1-1B	8943.5	5.12	8.26E+03	6.88E+02	6.88E+02	2.88E+03	1.21E-07
D1-2A	6944.9	1.37	6.17E+03	7.72E+02	7.72E+02	1.81E+03	3.04E-07
D1-2B	6285.4	2.29	6.68E+03	-3.98E+02	3.98E+02	2.07E+03	2.32E-07
D2-1A	10470.6	3.03	7.09E+03	3.38E+03	3.38E+03	2.28E+03	1.92E-07
D2-1B	8782.1	3.22	7.20E+03	1.58E+03	1.58E+03	2.34E+03	1.83E-07
EC-1A	8337.3	4.49	7.91E+03	4.32E+02	4.32E+02	2.70E+03	1.37E-07
EC-1B	7319.9	4.58	7.96E+03	-6.36E+02	6.36E+02	2.73E+03	1.35E-07
EC-2A	9803.0	12.6	1.24E+04	-2.61E+03	2.61E+03	5.00E+03	3.99E-08
EC-2B	3760.2	5.67	8.56E+03	-4.80E+03	4.80E+03	3.03E+03	1.09E-07
EC-3A	9343.7	24.4	1.90E+04	-9.62E+03	9.62E+03	8.36E+03	1.43E-08
EC-3B	31228.4	22.1	1.77E+04	1.35E+04	1.35E+04	7.70E+03	1.69E-08
EC-4A	26257.2	28.8	2.14E+04	4.85E+03	4.85E+03	9.61E+03	1.08E-08
EC-4B	9798.3	7.66	9.67E+03	1.32E+02	1.32E+02	3.60E+03	7.71E-08
LC-1A	6838.7	0.721	5.81E+03	1.03E+03	1.03E+03	1.63E+03	3.77E-07
LC-1B	15393.8	0.964	5.95E+03	9.45E+03	9.45E+03	1.70E+03	3.47E-07
MC-1A	10308.4	9.35	1.06E+04	-2.96E+02	2.96E+02	4.08E+03	6.01E-08
MC-1B	10040.3	2.86	7.00E+03	3.04E+03	3.04E+03	2.24E+03	2.00E-07
MC-2A	8594.3	4.98	8.18E+03	4.17E+02	4.17E+02	2.84E+03	1.24E-07
MC-2B	9115.8	14.2	1.33E+04	-4.18E+03	4.18E+03	5.46E+03	3.36E-08
MC-3A	5032.9	5.68	8.57E+03	-3.53E+03	3.53E+03	3.04E+03	1.08E-07
MC-3B	6018.3	18	1.54E+04	-9.39E+03	9.39E+03	6.54E+03	2.34E-08
PC-1A	40766.3	31.1	2.27E+04	1.81E+04	1.81E+04	1.03E+04	9.50E-09
PC-1B	18360.8	24.5	1.90E+04	-6.58E+02	6.58E+02	8.39E+03	1.42E-08
PC-2A	3534.4	1.24	6.10E+03	-2.57E+03	2.57E+03	1.78E+03	3.17E-07
PC-2B	3473.3	1.03	5.98E+03	-2.51E+03	2.51E+03	1.72E+03	3.39E-07
PC-3A	1691.0	1.89	6.46E+03	-4.77E+03	4.77E+03	1.96E+03	2.60E-07
PC-3B	1127.6	0.604	5.75E+03	-4.62E+03	4.62E+03	1.60E+03	3.93E-07

OVERALL FIT

Multiple R	0.468915311	AIC	27.57921118
R Square	0.219881568	AICc	28.05921118
Adjusted R Square	0.190982293	BSC	28.91141569
Standard Error	1.638572792		
Observations	28		

ANOVA (Alpha 0.05)

	df	SS	MS	F	p-value	sig
Regression	1	19.67583237	19.67583	7.328272925	0.011833	yes
Residual	26	69.80794059	2.684921			
Total	27	89.48377306				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	**5411.78835**	993.7253322	5.44596	1.03989E-05	3369.157	7454.42	
X-Ar1268 (mg/kg)	**555.3770261**	205.1573558	2.707078	0.011833315	133.67	977.084	1

Location	PCDD/F [ng/kg]	Ar1268 [mg/kg]	Pred Y	Residual	ABS(Res)	Pred Y'	Weight	Weight * X	Weight*X^2
D1-1A	8114.0	2.29	6683.60	1430.398	1430.40	2074.261752	2.3242E-07	5.32241E-07	1.21883E-06
D1-1B	8943.5	5.12	8255.32	688.181	688.18	2878.455926	1.20693E-07	6.17946E-07	3.16389E-06
D1-2A	6944.9	1.37	6172.65	772.245	772.25	1812.827604	3.04296E-07	4.16877E-07	5.71121E-07
D1-2B	6285.4	2.29	6683.60	-398.202	398.20	2074.261752	2.3242E-07	5.32241E-07	1.21883E-06
D2-1A	10470.6	3.03	7094.58	3376.019	3376.02	2284.545741	1.91602E-07	5.80554E-07	1.75908E-06
D2-1B	8782.1	3.22	7200.10	1581.998	1582.00	2338.537576	1.82857E-07	5.88799E-07	1.89593E-06
EC-1A	8337.3	4.49	7905.43	431.869	431.87	2699.430367	1.37232E-07	6.16172E-07	2.76661E-06
EC-1B	7319.9	4.58	7955.42	-635.515	635.52	2725.905447	1.34468E-07	6.16781E-07	2.82486E-06
EC-2A	9803.0	12.6	12409.54	-2606.539	2606.54	5004.029219	3.99356E-08	5.03189E-07	6.34018E-06
EC-2B	3760.2	5.67	8560.78	-4800.576	4800.58	3034.748079	1.08581E-07	6.15656E-07	3.49077E-06
EC-3A	9343.7	24.4	18962.99	-9619.288	9619.29	8357.206338	1.43178E-08	3.49355E-07	8.52427E-06
EC-3B	31228.4	22.1	17685.62	13542.779	13542.78	7703.620968	1.68504E-08	3.72394E-07	8.2295E-06
EC-4A	26257.2	28.8	21406.65	4850.553	4850.55	9607.54357	1.08337E-08	3.12009E-07	8.98587E-06
EC-4B	9798.3	7.66	9665.98	132.324	132.32	3600.241509	7.71501E-08	5.9097E-07	4.52683E-06
LC-1A	6838.7	0.721	5812.22	1026.485	1026.48	1628.402862	3.77117E-07	2.71901E-07	1.96041E-07
LC-1B	15393.8	0.964	5947.17	9446.628	9446.63	1697.455577	3.47059E-07	3.34505E-07	3.2252E-07
MC-1A	10308.4	9.35	10604.56	-296.164	296.16	4080.484673	6.00588E-08	5.6155E-07	5.25049E-06
MC-1B	10040.3	2.86	7000.17	3040.133	3040.13	2236.237257	1.9997E-07	5.71913E-07	1.63567E-06
MC-2A	8594.3	4.98	8177.57	416.734	416.73	2838.672468	1.24099E-07	6.18015E-07	3.07771E-06
MC-2B	9115.8	14.2	13298.14	-4182.342	4182.34	5458.697303	3.356E-08	4.76552E-07	6.76704E-06
MC-3A	5032.9	5.68	8566.33	-3533.430	3533.43	3037.589755	1.08978E-07	6.15588E-07	3.49654E-06
MC-3B	6018.3	18	15408.57	-9390.275	9390.27	6538.534002	2.33905E-08	4.21029E-07	7.57852E-06
PC-1A	40766.3	31.1	22684.01	18082.286	18082.29	10261.12894	9.49751E-09	2.95373E-07	9.18609E-06
PC-1B	18360.8	24.5	19018.53	-657.725	657.73	8385.623094	1.4221E-08	3.48414E-07	8.53614E-06
PC-2A	3534.4	1.24	6100.46	-2566.056	2566.06	1775.885822	3.17081E-07	3.9318E-07	4.87543E-07
PC-2B	3473.3	1.03	5983.83	-2510.527	2510.53	1716.210636	3.39515E-07	3.497E-07	3.60191E-07
PC-3A	1691.0	1.89	6461.45	-4770.451	4770.45	1960.594731	2.6015E-07	4.91584E-07	9.29283E-07
PC-3B	1127.6	0.604	5747.24	-4619.646	4619.67	1595.159258	3.93901E-07	2.37373E-07	1.43373E-07
						SUM	4.41095E-06	1.2232E-05	0.000103484

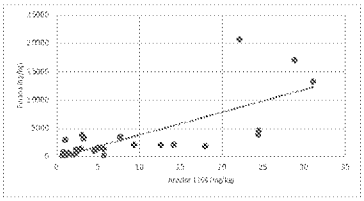
WLS Error Variance 15876

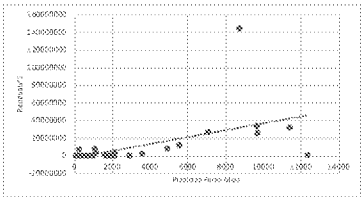
$$Var = \frac{\sum w_i}{\left(\left(\sum w_i\right)\left(\sum w_i x_i^2\right) - \left(\sum w_i x_i\right)^2\right)}$$

WLS Var:OLS Var =	1.02
Heteroscedasticity not severe	

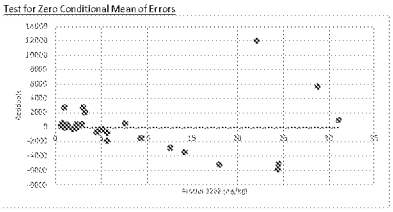
Case 1b: Furan Congener Concentration and Aroclor 1268 (Co-location Study Data)

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred PCDD/F (ng/kg)	Pred PCDD/F^2	Residual PCDD/F	Residual^2
D1-1A	1206.0	2.29	749.82	562232.36	456.18	208098.77
D1-1B	1641.0	5.12	1888.07	3564802.53	-247.07	61042.83
D1-2A	564.5	1.37	379.79	144241.02	184.71	34117.50
D1-2B	600.4	2.29	749.82	562232.36	-149.42	22326.80
D2-1A	3831.0	3.03	1047.46	1097162.02	2783.54	7748122.64
D2-1B	3162.0	3.22	1123.87	1263093.73	2038.13	4153955.85
EC-1A	999.2	4.49	1634.68	2672171.55	-635.48	403832.05
EC-1B	1001.7	4.58	1670.88	2791828.20	-669.18	447797.16
EC-2A	2030.0	12.6	4896.58	23976493.15	-2866.58	8217279.41
EC-2B	229.9	5.67	2109.28	4449072.79	-1879.38	3532078.70
EC-3A	3810.0	24.4	9642.63	92980254.24	-5832.63	34019536.98
EC-3B	20737.0	22.1	8717.55	75995676.97	12019.45	144467179.73
EC-4A	17065.0	28.8	11412.34	130241491.73	5652.66	31952571.29
EC-4B	3446.0	7.66	2909.68	8466209.98	536.32	287644.25
LC-1A	728.2	0.721	118.76	14103.50	609.44	371419.36
LC-1B	2958.0	0.964	216.49	46869.89	2741.51	7515852.10
MC-1A	2089.0	9.35	3589.41	12883833.45	-1500.41	2251217.34
MC-1B	1409.0	2.86	979.08	958597.19	429.92	184831.41
MC-2A	1515.0	4.98	1831.76	3355342.62	-316.76	100336.54
MC-2B	2089.0	14.2	5540.11	30692836.13	-3451.11	11910171.02
MC-3A	1358.0	5.68	2113.30	4466056.35	-755.30	570485.05
MC-3B	1872.0	18	7068.50	49963687.21	-5196.50	27003608.54
PC-1A	13310.0	31.1	12337.42	152211844.57	972.58	945918.77
PC-1B	4611.0	24.5	9682.85	93757539.11	-5071.85	25723638.84
PC-2A	649.3	1.24	327.50	107258.74	321.80	103552.80
PC-2B	206.7	1.03	243.04	59068.56	-36.34	1320.61
PC-3A	316.2	1.89	588.94	346848.67	-272.74	74386.34
PC-3B	206.2	0.604	71.70	5140.87	134.50	18090.28





Test for Zero Conditional Mean of Errors



No discernable relationship between residuals and independent variable
Cov(ûᵢ , xᵢ) = 0

Tests for Homoscedasticity

BREUSCH-PAGAN SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.523793041
R Square	0.27435915
Adjusted R Square	0.246449887
Standard Error	24392362.78
Observations	28

$$\hat{u}^2 = d_0 + x d_1$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p<0.05
Status: Heteroscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	5.84896E+15	5.84896E+15	9.830397364	0.004226849
Residual	26	1.54697E+16	5.94987E+14		
Total	27	2.13186E+16			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-2557452.391	6354221.956	-0.402480809	0.690620244	-15618742.68	10503837.9	-15618742.68	10503837.9
Ar1268 (mg/kg)	1568769.505	500349.6519	3.13534645	0.004226849	540286.0659	2597252.944	540286.0659	2597252.944

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.555929352
R Square	0.309057444
Adjusted R Square	0.25378204
Standard Error	24273402.05
Observations	28

$$\hat{u}^2 = d_0 + \hat{Y} \times d_1 + \hat{Y}^2 \times d_2$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p<0.05
Status: Heteroscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	2	6.58868E+15	3.29434E+15	5.591229002	0.009840661
Residual	25	1.473E+16	5.89198E+14		
Total	27	2.13186E+16			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-7701076.211	8067482.045	-0.95458238	0.348928743	-24316366.51	8914214.085	-24316366.51	8914214.085
Pred PCDD/F (ng/kg)	9217.380159	4904.100051	1.879525308	0.07187753	-882.8029632	19317.56328	-882.8029632	19317.56328
Pred PCDD/F^2	-0.480432373	0.428774714	-1.120477391	0.273159218	-1.363510427	0.402645681	-1.363510427	0.402645681

Location	Y: Furans (ng/kg)	X: Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight	Weight * X	Weight *X^2
D1-1A	1206.0	2.29	749.82	456.178	456.18	806.5988312	1.53704E-06	3.51982E-06	8.06039E-06
D1-1B	1641.0	5.12	1888.07	-247.068	247.07	1357.759577	5.42443E-07	2.77731E-06	1.42198E-05
D1-2A	564.5	1.37	379.79	184.709	184.71	627.4228998	2.54027E-06	3.48017E-06	4.76783E-06
D1-2B	600.4	2.29	749.82	-149.422	149.42	806.5988312	1.53704E-06	3.51982E-06	8.06039E-06
D2-1A	3831.0	3.03	1047.46	2783.545	2783.54	950.718602	1.10636E-06	3.35227E-06	1.01574E-05
D2-1B	3162.0	3.22	1123.87	2038.126	2038.13	987.722327	1.02502E-06	3.30055E-06	1.06278E-05
EC-1A	999.2	4.49	1634.68	-635.478	635.48	1235.063015	6.55574E-07	2.94353E-06	1.32164E-05
EC-1B	1001.7	4.58	1670.88	-669.176	669.18	1252.591095	6.37355E-07	2.91909E-06	1.33694E-05
EC-2A	2030.0	12.6	4896.58	-2866.580	2866.58	2814.537801	1.26237E-07	1.59058E-06	2.00413E-05
EC-2B	229.9	5.67	2109.28	-1879.383	1879.38	1464.875622	4.66013E-07	2.6423E-06	1.49818E-05
EC-3A	3810.0	24.4	9642.63	-5832.627	5832.63	5112.663877	3.82565E-08	9.33459E-07	2.27764E-05
EC-3B	20737.0	22.1	8717.55	12019.450	12019.45	4664.724049	4.59566E-08	1.01564E-06	2.24457E-05
EC-4A	17065.0	28.8	11412.34	5652.661	5652.66	5969.592244	2.80615E-08	8.08171E-07	2.32753E-05
EC-4B	3446.0	7.66	2909.68	536.325	536.32	1852.440952	2.91415E-07	2.23224E-06	1.70989E-05
LC-1A	728.2	0.721	118.76	609.442	609.44	501.0259656	3.98363E-06	2.8722E-06	2.07086E-06
LC-1B	2958.0	0.964	216.49	2741.505	2741.51	548.3517823	3.32569E-06	3.20596E-06	3.09055E-06
MC-1A	2089.0	9.35	3589.41	-1500.406	1500.41	2181.579348	2.10115E-07	1.96458E-06	1.83688E-05
MC-1B	1409.0	2.86	979.08	429.920	429.92	917.610006	1.18764E-06	3.39664E-06	9.7144E-06
MC-2A	1515.0	4.98	1831.76	-316.759	316.76	1330.493674	5.64904E-07	2.81322E-06	1.40098E-05
MC-2B	2089.0	14.2	5540.11	-3451.112	3451.11	3126.148116	1.02325E-07	1.45301E-06	2.06328E-05
MC-3A	1358.0	5.68	2113.30	-755.305	755.30	1466.823187	4.64777E-07	2.63993E-06	1.49948E-05
MC-3B	1872.0	18	7068.50	-5196.500	5196.50	3866.222615	6.69E-08	1.2042E-06	2.16756E-05
PC-1A	13310.0	31.1	12337.42	972.584	972.58	6417.532073	2.42809E-08	7.55134E-07	2.34847E-05
PC-1B	4611.0	24.5	9682.85	-5071.848	5071.85	5132.139522	3.79667E-08	9.30185E-07	2.27895E-05
PC-2A	649.3	1.24	327.50	321.796	321.80	602.1045617	2.75839E-06	3.42041E-06	4.24131E-06
PC-2B	206.7	1.03	243.04	-36.340	36.34	561.2057078	3.17509E-06	3.27034E-06	3.36845E-06
PC-3A	316.2	1.89	588.94	-272.739	272.74	728.6962523	1.88325E-06	3.55933E-06	6.72714E-06
PC-3B	206.2	0.604	71.70	134.500	134.50	478.2394613	4.37229E-06	2.64086E-06	1.59508E-06
						SUM	3.27343E-05	6.91609E-05	0.000369863

$$Var = \frac{\sum w_i}{\left(\left(\sum w_i\right)\left(\sum w_i x_i^2\right) - \left(\sum w_i x_i\right)^2\right)}$$

Error Variance of OLS **4469**

Case 1b: Furan Congener Concentration and Aroclor 1268 (Co-location Study Data)

Location	Furans (mg/kg)	Ar1268 (mg/kg)
D1-1A	1206.0	2.29
D1-1B	1641.0	5.12
D1-2A	564.5	1.37
D1-2B	600.4	2.29
D2-1A	3831.0	3.03
D2-1B	3162.0	3.22
EC-1A	999.2	4.49
EC-1B	1001.7	4.58
EC-2A	2030.0	12.6
EC-2B	229.9	5.67
EC-3A	3810.0	24.4
EC-3B	20737.0	22.1
EC-4A	17065.0	28.8
EC-4B	3446.0	7.66
LC-1A	728.2	0.721
LC-1B	2958.0	0.964
MC-1A	2089.0	9.35
MC-1B	1409.0	2.86
MC-2A	1515.0	4.98
MC-2B	2089.0	14.2
MC-3A	1358.0	5.68
MC-3B	1872.0	18
PC-1A	13310.0	31.1
PC-1B	4611.0	24.5
PC-2A	649.3	1.24
PC-2B	206.7	1.03
PC-3A	316.2	1.89
PC-3B	206.2	0.604

Weighted Least Squares performed with "Real Stats" Add-In

$$Pred\ Y_i' = Abs(Res)x + \partial_1$$

$$W_i = \frac{1}{Pred\ Y_i'^2}$$

WLS solution is asymptotic at Iteration #4.

Iteration #1

Location	Y-Furans (mg/kg)	X-Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight
D1-1A	1206.0	2.29	7.50E+02	4.56E+02	4.56E+02	8.07E+02	1.54E-06
D1-1B	1641.0	5.12	1.89E+03	-2.47E+02	2.47E+02	1.36E+03	5.42E-07
D1-2A	564.5	1.37	3.80E+02	1.85E+02	1.85E+02	6.27E+02	2.54E-06
D1-2B	600.4	2.29	7.50E+02	-1.49E+02	1.49E+02	8.07E+02	1.54E-06
D2-1A	3831.0	3.03	1.05E+03	2.78E+03	2.78E+03	9.51E+02	1.11E-06
D2-1B	3162.0	3.22	1.12E+03	2.04E+03	2.04E+03	9.88E+02	1.01E-06
EC-1A	999.2	4.49	1.63E+03	-6.35E+02	6.35E+02	1.24E+03	6.56E-07
EC-1B	1001.7	4.58	1.67E+03	-6.69E+02	6.69E+02	1.25E+03	6.37E-07
EC-2A	2030.0	12.6	4.90E+03	-2.87E+03	2.87E+03	2.81E+03	1.26E-07
EC-2B	229.9	5.67	2.11E+03	-1.88E+03	1.88E+03	1.46E+03	4.66E-07
EC-3A	3810.0	24.4	9.64E+03	-5.83E+03	5.83E+03	5.11E+03	3.83E-08
EC-3B	20737.0	22.1	8.72E+03	1.20E+04	1.20E+04	4.66E+03	4.60E-08
EC-4A	17065.0	28.8	1.14E+04	5.65E+03	5.65E+03	5.97E+03	2.81E-08
EC-4B	3446.0	7.66	2.91E+03	5.36E+02	5.36E+02	1.85E+03	2.91E-07
LC-1A	728.2	0.721	1.19E+02	6.09E+02	6.09E+02	5.01E+02	3.98E-06
LC-1B	2958.0	0.964	2.16E+02	2.74E+03	2.74E+03	5.48E+02	3.33E-06
MC-1A	2089.0	9.35	3.59E+03	-1.50E+03	1.50E+03	2.18E+03	2.10E-07
MC-1B	1409.0	2.86	9.79E+02	4.30E+02	4.30E+02	9.18E+02	1.19E-06
MC-2A	1515.0	4.98	1.83E+03	-3.17E+02	3.17E+02	1.33E+03	5.65E-07
MC-2B	2089.0	14.2	5.54E+03	-3.45E+03	3.45E+03	3.13E+03	1.02E-07
MC-3A	1358.0	5.68	2.11E+03	-7.55E+02	7.55E+02	1.47E+03	4.05E-07
MC-3B	1872.0	18	7.07E+03	-5.20E+03	5.20E+03	3.87E+03	6.69E-08
PC-1A	13310.0	31.1	1.23E+04	9.73E+02	9.73E+02	6.42E+03	2.43E-08
PC-1B	4611.0	24.5	9.68E+03	-5.07E+03	5.07E+03	5.13E+03	3.80E-08
PC-2A	649.3	1.24	3.28E+02	3.22E+02	3.22E+02	6.02E+02	2.76E-06
PC-2B	206.7	1.03	2.43E+02	-3.63E+01	3.63E+01	5.01E+02	3.18E-06
PC-3A	316.2	1.89	5.89E+02	-2.73E+02	2.73E+02	7.29E+02	1.88E-06
PC-3B	206.2	0.604	7.17E+01	1.35E+02	1.35E+02	4.78E+02	4.37E-06

OVERALL FIT

Multiple R	0.531404882	AIC	16.49068942
R Square	0.282391149	AICc	16.97068942
Adjusted R Square	0.255813043	BSC	17.82289393
Standard Error	1.344223196		
Observations	28		

ANOVA (Alpha 0.05)

	df	SS	MS	F	p-value	sig
Regression	1	1.85E+01	18.48755215	10.23143716	0.003614717	yes
Residual	26	46.98033605	1.806936002			
Total	27	65.4678882				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	551.6392391	302.0778612	1.826149182	0.079333467	-69.2906974	1172.569176	
X-Ar1268 (mg/kg)	287.4539679	89.86694686	3.198661776	0.003614717	102.729813	472.1781227	1

Iteration #2

Location	Y-Furans (mg/kg)	X-Ar1268 (mg/kg)	Pred Y2	Residual	ABS(Res)	Pred Y2'	Weight
D1-1A	1206.0	2.29	1.21E+03	-3.91E+00	3.91E+00	6.62E+02	2.28E-06
D1-1B	1641.0	5.12	2.02E+03	-3.82E+02	3.82E+02	1.28E+03	6.12E-07
D1-2A	564.5	1.37	9.45E+02	-3.81E+02	3.81E+02	4.62E+02	4.68E-06
D1-2B	600.4	2.29	1.21E+03	-6.10E+02	6.10E+02	6.62E+02	2.28E-06
D2-1A	3831.0	3.03	1.42E+03	2.41E+03	2.41E+03	8.23E+02	1.48E-06
D2-1B	3162.0	3.22	1.48E+03	1.68E+03	1.68E+03	8.65E+02	1.34E-06
EC-1A	999.2	4.49	1.84E+03	-8.43E+02	8.43E+02	1.14E+03	7.68E-07
EC-1B	1001.7	4.58	1.87E+03	-8.66E+02	8.66E+02	1.16E+03	7.43E-07
EC-2A	2030.0	12.6	4.17E+03	-2.14E+03	2.14E+03	2.90E+03	1.19E-07
EC-2B	229.9	5.67	2.18E+03	-1.95E+03	1.95E+03	1.40E+03	5.12E-07
EC-3A	3810.0	24.4	7.57E+03	-3.76E+03	3.76E+03	5.47E+03	3.34E-08
EC-3B	20737.0	22.1	6.90E+03	1.38E+04	1.38E+04	4.97E+03	4.05E-08
EC-4A	17065.0	28.8	8.83E+03	8.23E+03	8.23E+03	6.43E+03	2.42E-08
EC-4B	3446.0	7.66	2.75E+03	6.92E+02	6.92E+02	1.83E+03	2.99E-07
LC-1A	728.2	0.721	7.59E+02	-3.07E+01	3.07E+01	3.21E+02	9.69E-06
LC-1B	2958.0	0.964	8.29E+02	2.13E+03	2.13E+03	3.74E+02	7.15E-06
MC-1A	2089.0	9.35	3.24E+03	-1.15E+03	1.15E+03	2.20E+03	2.07E-07
MC-1B	1409.0	2.86	1.37E+03	3.52E+01	3.52E+01	7.86E+02	1.62E-06
MC-2A	1515.0	4.98	1.98E+03	-4.68E+02	4.68E+02	1.25E+03	6.43E-07
MC-2B	2089.0	14.2	4.63E+03	-2.54E+03	2.54E+03	3.25E+03	9.45E-08
MC-3A	1358.0	5.68	2.18E+03	-8.26E+02	8.26E+02	1.40E+03	5.10E-07
MC-3B	1872.0	18	5.73E+03	-3.85E+03	3.85E+03	4.08E+03	6.01E-08
PC-1A	13310.0	31.1	9.49E+03	3.82E+03	3.82E+03	6.93E+03	2.08E-08
PC-1B	4611.0	24.5	7.59E+03	-2.98E+03	2.98E+03	5.49E+03	3.31E-08
PC-2A	649.3	1.24	9.08E+02	-2.59E+02	2.59E+02	4.34E+02	5.31E-06
PC-2B	206.7	1.03	8.48E+02	-6.41E+02	6.41E+02	3.88E+02	6.83E-06
PC-3A	316.2	1.89	1.09E+03	-7.79E+02	7.79E+02	5.75E+02	3.02E-06
PC-3B	206.2	0.604	7.25E+02	-5.19E+02	5.19E+02	2.96E+02	1.14E-05

OVERALL FIT

Multiple R	0.46308569	AIC	27.98762273
R Square	0.214448356	AICc	28.46762273
Adjusted R Square	0.185353851	BSC	29.31982724
Standard Error	1.65056869		
Observations	28		

ANOVA (Alpha 0.05)

	df	SS	MS	F	p-value	sig
Regression	1	19.33692805	19.33693	7.097760293	0.013078	yes
Residual	26	70.83363039	2.72437			
Total	27	90.17055843				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	560.4069157	274.0215026	2.04512	0.051087655	-2.85235	1123.666	
X-Ar1268 (mg/kg)	285.127461	107.023311	2.664162	0.013078081	65.13789	505.117	1

Iteration #3

Location	Y-Furans (mg/kg)	X-Ar1268 (mg/kg)	Pred Y3	Residual	ABS(Res)	Pred Y3'	Weight
D1-1A	1206.0	2.29	1.21E+03	-7.35E+00	7.35E+00	6.60E+02	2.30E-06
D1-1B	1641.0	5.12	2.02E+03	-3.79E+02	3.79E+02	1.28E+03	6.14E-07
D1-2A	564.5	1.37	9.51E+02	-3.87E+02	3.87E+02	4.59E+02	4.74E-06
D1-2B	600.4	2.29	1.21E+03	-6.13E+02	6.13E+02	6.60E+02	2.30E-06
D2-1A	3831.0	3.03	1.42E+03	2.41E+03	2.41E+03	8.21E+02	1.48E-06
D2-1B	3162.0	3.22	1.48E+03	1.68E+03	1.68E+03	8.63E+02	1.34E-06
EC-1A	999.2	4.49	1.84E+03	-8.41E+02	8.41E+02	1.14E+03	7.71E-07
EC-1B	1001.7	4.58	1.87E+03	-8.65E+02	8.65E+02	1.16E+03	7.45E-07
EC-2A	2030.0	12.6	4.15E+03	-2.12E+03	2.12E+03	2.91E+03	1.18E-07
EC-2B	229.9	5.67	2.18E+03	-1.95E+03	1.95E+03	1.40E+03	5.13E-07
EC-3A	3810.0	24.4	7.52E+03	-3.71E+03	3.71E+03	5.48E+03	3.33E-08
EC-3B	20737.0	22.1	6.86E+03	1.39E+04	1.39E+04	4.98E+03	4.04E-08
EC-4A	17065.0	28.8	8.77E+03	8.29E+03	8.29E+03	6.44E+03	2.41E-08
EC-4B	3446.0	7.66	2.74E+03	7.02E+02	7.02E+02	1.83E+03	2.99E-07
LC-1A	728.2	0.721	7.66E+02	-3.78E+01	3.78E+01	3.18E+02	9.88E-06
LC-1B	2958.0	0.964	8.35E+02	2.12E+03	2.12E+03	3.71E+02	7.26E-06
MC-1A	2089.0	9.35	3.23E+03	-1.14E+03	1.14E+03	2.20E+03	2.07E-07
MC-1B	1409.0	2.86	1.38E+03	3.31E+01	3.31E+01	7.84E+02	1.63E-06
MC-2A	1515.0	4.98	1.98E+03	-4.65E+02	4.65E+02	1.25E+03	6.44E-07
MC-2B	2089.0	14.2	4.61E+03	-2.52E+03	2.52E+03	3.25E+03	9.44E-08
MC-3A	1358.0	5.68	2.18E+03	-8.22E+02	8.22E+02	1.40E+03	5.11E-07
MC-3B	1872.0	18	5.69E+03	-3.82E+03	3.82E+03	4.08E+03	6.00E-08
PC-1A	13310.0	31.1	9.43E+03	3.88E+03	3.88E+03	6.94E+03	2.08E-08
PC-1B	4611.0	24.5	7.55E+03	-2.94E+03	2.94E+03	5.50E+03	3.31E-08
PC-2A	649.3	1.24	9.14E+02	-2.65E+02	2.65E+02	4.31E+02	5.38E-06
PC-2B	206.7	1.03	8.54E+02	-6.47E+02	6.47E+02	3.85E+02	6.73E-06
PC-3A	316.2	1.89	1.10E+03	-7.83E+02	7.83E+02	5.73E+02	3.05E-06
PC-3B	206.2	0.604	7.33E+02	-5.26E+02	5.26E+02	2.93E+02	1.17E-05

OVERALL FIT

Multiple R	0.461657127	AIC	28.27490375
R Square	0.213127303	AICc	28.75490375
Adjusted R Square	0.18398387	BSC	29.60710826
Standard Error	1.659055884		
Observations	28		

ANOVA (Alpha 0.05)

	df	SS	MS	F	p-value	sig
Regression	1	19.38340151	19.38340151	7.042193622	0.013399179	yes
Residual	26	71.56412706	2.752466425			
Total	27	90.94752857				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	560.1442921	273.5617429	2.047987321	0.05082694	-2.189923803	1122.458508	
X-Ar1268 (mg/kg)	285.208369	107.4752055	2.653713176	0.013399179	64.28992015	506.1258179	1

Iteration #4

Location	Y-Furans (mg/kg)	X-Ar1268 (mg/kg)	Pred Y4	Residual	ABS(Res)	Pred Y4'	Weight
D1-1A	1206.0	2.29	1.21E+03	-7.27E+00	7.27E+00	6.60E+02	2.30E-06
D1-1B	1641.0	5.12	2.02E+03	-3.79E+02	3.79E+02	1.28E+03	6.14E-07
D1-2A	564.5	1.37	9.51E+02	-3.89E+02	3.89E+02	4.60E+02	4.73E-06
D1-2B	600.4	2.29	1.21E+03	-6.13E+02	6.13E+02	6.60E+02	2.30E-06
D2-1A	3831.0	3.03	1.42E+03	2.41E+03	2.41E+03	8.21E+02	1.48E-06
D2-1B	3162.0	3.22	1.48E+03	1.68E+03	1.68E+03	8.63E+02	1.34E-06
EC-1A	999.2	4.49	1.84E+03	-8.42E+02	8.42E+02	1.14E+03	7.70E-07
EC-1B	1001.7	4.58	1.87E+03	-8.65E+02	8.65E+02	1.16E+03	7.45E-07
EC-2A	2030.0	12.6	4.15E+03	-2.12E+03	2.12E+03	2.91E+03	1.18E-07
EC-2B	229.9	5.67	2.18E+03	-1.95E+03	1.95E+03	1.40E+03	5.13E-07
EC-3A	3810.0	24.4	7.52E+03	-3.71E+03	3.71E+03	5.48E+03	3.33E-08
EC-3B	20737.0	22.1	6.86E+03	1.39E+04	1.39E+04	4.98E+03	4.04E-08
EC-4A	17065.0	28.8	8.77E+03	8.29E+03	8.29E+03	6.44E+03	2.41E-08
EC-4B	3446.0	7.66	2.74E+03	7.01E+02	7.01E+02	1.83E+03	2.99E-07
LC-1A	728.2	0.721	7.66E+02	-3.76E+01	3.76E+01	3.18E+02	9.88E-06
LC-1B	2958.0	0.964	8.35E+02	2.12E+03	2.12E+03	3.71E+02	7.26E-06
MC-1A	2089.0	9.35	3.23E+03	-1.14E+03	1.14E+03	2.20E+03	2.07E-07
MC-1B	1409.0	2.86	1.38E+03	3.32E+01	3.32E+01	7.84E+02	1.63E-06
MC-2A	1515.0	4.98	1.98E+03	-4.65E+02	4.65E+02	1.25E+03	6.44E-07
MC-2B	2089.0	14.2	4.61E+03	-2.52E+03	2.52E+03	3.25E+03	9.44E-08
MC-3A	1358.0	5.68	2.18E+03	-8.22E+02	8.22E+02	1.40E+03	5.11E-07
MC-3B	1872.0	18	5.69E+03	-3.82E+03	3.82E+03	4.08E+03	6.00E-08
PC-1A	13310.0	31.1	9.43E+03	3.88E+03	3.88E+03	6.94E+03	2.08E-08
PC-1B	4611.0	24.5	7.55E+03	-2.94E+03	2.94E+03	5.50E+03	3.31E-08
PC-2A	649.3	1.24	9.14E+02	-2.65E+02	2.65E+02	4.31E+02	5.38E-06
PC-2B	206.7	1.03	8.54E+02	-6.47E+02	6.47E+02	3.86E+02	6.73E-06
PC-3A	316.2	1.89	1.10E+03	-7.83E+02	7.83E+02	5.73E+02	3.05E-06
PC-3B	206.2	0.604	7.32E+02	-5.26E+02	5.26E+02	2.93E+02	1.17E-05

OVERALL FIT

Multiple R	0.46171782	AIC	28.26210361
R Square	0.213183345	AICc	28.74210361
Adjusted R Square	0.184041988	BSC	29.59436812
Standard Error	1.658678487		
Observations	28		

ANOVA (Alpha 0.05)

	df	SS	MS	F	p-value	sig
Regression	1	1.94E+01	19.38106	7.044547098	0.013385	yes
Residual	26	71.53157244	2.751214			
Total	27	90.91263133				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	**560.1558712**	273.5812057	2.047494	0.050837793	-2.19935	1122.51	
X-Ar1268 (mg/kg)	**285.2047958**	107.4559048	2.654157	0.013385405	64.32602	506.0836	1

Location	Furans (mg/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight	Weight * X	Weight*X^2
D1-1A	1206.0	2.29	1213.27	-7.275	7.27	660.0074438	2.29563E-06	5.257E-06	1.20385E-05
D1-1B	1641.0	5.12	2020.40	-379.404	379.40	1276.525244	6.13681E-07	3.14205E-06	1.60872E-05
D1-2A	564.5	1.37	950.89	-386.386	386.39	459.5853401	4.73443E-06	6.48617E-06	8.88605E-06
D1-2B	600.4	2.29	1213.27	-612.875	612.87	660.0074438	2.29563E-06	5.257E-06	1.20385E-05
D2-1A	3831.0	3.03	1424.33	2406.674	2406.67	821.2165225	1.48281E-06	4.49291E-06	1.36135E-05
D2-1B	3162.0	3.22	1478.52	1683.485	1683.48	862.6080426	1.34392E-06	4.32742E-06	1.39343E-05
EC-1A	999.2	4.49	1840.73	-841.525	841.53	1138.277678	7.70444E-07	3.45929E-06	1.55322E-05
EC-1B	1001.7	4.58	1866.39	-864.694	864.69	1158.884187	7.44595E-07	3.41024E-06	1.56189E-05
EC-2A	2030.0	12.6	4153.74	-2123.736	2123.74	2906.042039	1.18412E-07	1.49199E-06	1.87991E-05
EC-2B	229.9	5.67	2177.27	-1947.367	1947.37	1396.340803	5.12882E-07	2.90804E-06	1.64886E-05
EC-3A	3810.0	24.4	7519.15	-3709.153	3709.15	5476.673293	3.33401E-08	8.13497E-07	1.98493E-05
EC-3B	20737.0	22.1	8863.18	11873.818	11873.82	4575.610048	4.0393E-08	8.92685E-07	1.97283E-05
EC-4A	17065.0	28.8	8774.05	8290.946	8290.95	6435.21376	2.41478E-08	6.95451E-07	2.0029E-05
EC-4B	3446.0	7.66	2744.82	701.175	701.18	1829.862514	2.9865E-07	2.28766E-06	1.75235E-05
LC-1A	728.2	0.721	765.79	-37.589	37.59	318.2006272	9.87638E-06	7.12087E-06	5.13415E-06
LC-1B	2958.0	0.964	835.09	2122.907	2122.91	371.138203	7.25987E-06	6.99851E-06	6.74657E-06
MC-1A	2089.0	9.35	3226.82	-1137.821	1137.82	2198.029194	2.06982E-07	1.93528E-06	1.80949E-05
MC-1B	1409.0	2.86	1375.84	33.158	33.16	784.1820044	1.62617E-06	4.65085E-06	1.33014E-05
MC-2A	1515.0	4.98	1980.48	-465.476	465.48	1246.02423	6.44091E-07	3.20757E-06	1.59737E-05
MC-2B	2089.0	14.2	4610.06	-2521.064	2521.06	3254.602209	9.4407E-08	1.34058E-06	1.90362E-05
MC-3A	1358.0	5.68	2180.12	-822.119	822.12	1398.519304	5.11285E-07	2.9041E-06	1.64953E-05
MC-3B	1872.0	18	5693.84	-3821.842	3821.84	4082.432613	6.00815E-08	1.08003E-06	1.94405E-05
PC-1A	13310.0	31.1	9430.03	3879.975	3879.97	6936.269004	2.07845E-08	6.46411E-07	2.01034E-05
PC-1B	4611.0	24.5	7547.67	-2936.673	2936.67	5498.458303	3.30764E-08	8.10372E-07	1.98541E-05
PC-2A	649.3	1.24	913.81	-264.510	264.51	431.2648323	5.37665E-06	6.66705E-06	8.26714E-06
PC-2B	206.7	1.03	853.92	-647.217	647.22	385.51631	6.72844E-06	6.93029E-06	7.1382E-06
PC-3A	316.2	1.89	1099.19	-782.993	782.99	572.8674014	3.04714E-06	5.75909E-06	1.08847E-05
PC-3B	206.2	0.604	732.42	-526.220	526.22	292.7121647	1.16713E-05	7.04945E-06	4.25787E-06
						SUM	6.24655E-05	0.000102022	0.000404895

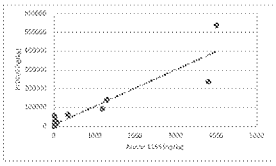
WLS Error Variance	4137

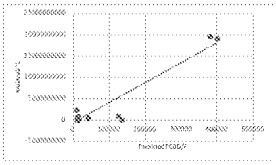
$$Var = \frac{\sum w_i}{\left(\left(\sum w_i\right)\left(\sum w_i x_i^2\right) - \left(\sum w_i x_i\right)^2\right)}$$

OLS Var:WLS Var =	1.1
Heteroscedasticity not severe	

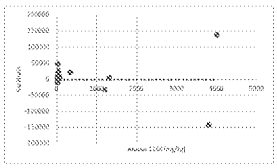
Case 2a: PCDD/F Concentration and Aroclor 1268 (Cumulative Data Set)

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)	Pred PCDD/F (ng/kg)	Pred PCDD/F^2	Residual PCDD/F	Residual^2
36	27038	55	15281.41	233521431.72	11756.49	138215069.49
61	141906	1300	136659.22	18675743689.94	5246.77	27528637.72
68	64192	330	42091.77	1771717029.84	22100.23	488420160.62
1718	18409	58	15378.90	236510573.31	3030.30	9182717.23
BR048	2981	1.4	10055.82	101119815.95	-7074.82	50053147.71
C-15	10834	0.099	9928.99	98584793.77	905.01	819047.46
C-6	59189	7.58	10658.33	113599931.55	48530.67	2355226152.32
C-8	10654	2.2	10133.82	102694281.63	520.58	271005.02
111	9396	6.1	10514.04	110545002.96	-1117.87	1249186.39
EPA-E3	240328	3600	380388.78	144696384863.54	-140061.58	19617246241.84
EPA-F2	94088	1188	125740.10	15810571169.02	-31652.40	1001874151.43
EPA-H1	538204	4000	399888.22	159910592187.68	138315.98	19131399048.03
GRID MARSH	5980	6.1	10514.04	110545002.96	-4534.04	20557505.00
117	2133	11	10991.75	120818573.87	-8858.34	78470130.23
110	3049	0.25	9943.71	98877346.21	-6895.11	47542526.41
109	856	1.1	10026.58	100532251.64	-9170.88	84104889.80
101	2058	0.085	9927.62	98557691.86	-7870.03	61937351.09
102	2678	0.13	9932.01	98644818.85	-7253.99	52620411.67
D1-1A	8114	2.29	10142.59	102872192.95	-2028.59	4115189.60
D1-1B	8944	5.12	10418.50	108545058.86	-1475.00	2175813.19
D1-2A	6945	1.37	10052.90	101060801.72	-3108.00	9659665.02
D1-2B	6285	2.29	10142.59	102872192.95	-3857.19	14877937.91
D2-1A	10471	3.03	10214.74	104340657.16	255.86	85465.75
D2-1B	8782	3.22	10233.26	104719626.10	-1451.16	2105867.60
EC-1A	8337	4.49	10357.08	107268921.15	-2019.78	4079494.58
EC-1B	7320	4.58	10365.85	107450850.32	-3045.95	9277812.61
EC-2A	9803	12.6	11147.74	124272058.50	-1344.74	1808319.80
EC-2B	3750	5.67	10472.12	109665228.60	-6711.92	45049826.06
EC-3A	9344	24.4	12298.15	151244396.97	-2954.45	8728751.41
EC-3B	31228	22.1	12073.91	145779397.61	19154.49	366894335.58
EC-4A	26257	28.8	12727.11	161976375.27	13530.09	183063286.17
EC-4B	9798	7.66	10666.13	113766249.01	-867.83	753122.39
LC-1A	6839	0.721	9989.63	99792661.83	-3150.93	9928345.45
LC-1B	15394	0.964	10013.32	100266543.83	5380.48	28949583.08
MC-1A	10308	9.35	10830.89	117306136.99	-522.49	272993.81
MC-1B	10040	2.86	10198.16	104002540.32	-157.86	24920.91
MC-2A	8594	4.98	10404.85	108258942.90	-1810.55	3278980.75
MC-2B	9116	14.2	11303.73	127774207.36	-2187.93	4787917.45
MC-3A	5033	5.68	10473.09	109685648.55	-5440.19	29595885.10
MC-3B	6018	18	11674.20	136286848.04	-5655.80	31988157.52
PC-1A	40766	31.1	12951.34	167737309.61	27814.96	773671781.14
PC-1B	18361	24.5	12307.90	151484285.83	6052.90	36637655.74
PC-2A	3534	1.24	10040.23	100806141.66	-6506.83	42325774.23
PC-2B	3473	1.03	10019.75	100395446.35	-6546.45	42856044.38
PC-3A	1691	1.89	10103.60	102082954.56	-8412.60	70771773.48
PC-3B	1128	0.604	9978.22	99584898.77	-8850.85	78334025.29





Test for Zero Conditional Mean of Errors



No discernable relationship between residuals and independent variable
$Cov(\hat{u}_i, x_i) = 0$

Tests for Homoscedasticity

BREUSCH-PAGAN SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.952125124
R Square	0.906542253
Adjusted R Square	0.934418213
Standard Error	1231917708
Observations	46

$$\hat{u}^2 = d_0 + x d_1$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p<0.05
Status: Heteroscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	6.47722E+20	6.47722E+20	426.8009898	2.82892E-24
Residual	44	6.67753E+19	1.51762E+18		
Total	45	7.14498E+20			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-115916071.8	189192582.4	-0.612688248	0.543236363	-497206667.8	265376524.1	-497206667.8	265376524.1
Ar1268 (mg/kg)	4589104.073	221185.9888	20.65916237	2.82892E-24	4123373.311	5014834.836	4123373.311	5014834.836

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.992172705
R Square	0.984406678
Adjusted R Square	0.983681405
Standard Error	509020774.5
Observations	46

$$\hat{u}^2 = d_0 + \hat{Y} \times d_1 + \hat{Y}^2 \times d_2$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p<0.05
Status: Heteroscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	2	7.09356E+20	3.51678E+20	1357.295189	1.40664E-39
Residual	43	1.11414E+19	2.59102E+17		
Total	45	7.14498E+20			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	308067879.8	101410211.4	3.038034094	0.004098814	103574497.5	512600862.2	103574497.5	512600862.2
Pred PCDD/F (ng/kg)	-19923.06467	4533.230476	-4.141548038	0.000158189	-28286.21674	-9759.952596	-28286.21674	-9759.952596
Pred PCDD/F^2	0.173239624	0.011822595	14.65326521	2.51397E-18	0.149397088	0.197082159	0.149397088	0.197082159

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y	Weight	Weight * X	Weight*X^2
36	27038	55	15281.41	11756.492	11756.49	7238.845451	1.90636E-08	1.0496E-06	5.7728E-05
61	141906	1300	136659.22	5246.774	5246.77	47203.59617	4.48797E-10	5.83436E-07	0.000758467
68	64192	330	42091.77	22100.230	22100.23	16066.40064	3.87408E-09	1.27843E-06	0.000421882
1718	18409	58	15378.90	3030.300	3030.30	7270.545863	1.89155E-08	1.09927E-06	5.53191E-05
BR048	2981	1.4	10055.82	-7074.825	7074.82	5518.274668	3.28393E-08	4.5975E-08	5.4365E-08
C-15	10834	0.099	9928.99	905.012	905.01	5476.512306	3.3342E-08	3.30085E-09	3.26785E-10
C-6	59189	7.58	10658.33	48530.672	48530.67	5716.653912	3.05996E-08	2.31945E-07	1.75814E-06
C-8	10654	2.2	10133.82	520.581	520.58	5543.954829	3.25357E-08	7.15786E-08	1.57473E-07
111	9396	6.1	10514.04	-1117.871	1117.87	5669.145614	3.11146E-08	1.89799E-07	1.15778E-06
EPA-E3	240328	3600	380388.78	-140061.580	140061.58	127454.0996	8.15591E-11	2.33925E-07	0.000688314
EPA-F2	94088	1188	125740.10	-31652.396	31652.40	43606.37351	5.25848E-10	6.24797E-07	0.000742152
EPA-H1	538204	4000	399888.22	138315.975	138315.98	133874.1399	5.57865E-11	2.23186E-07	0.000892743
GRID MARSH	5980	6.1	10514.04	-4534.038	4534.04	5669.145614	3.11146E-08	1.89799E-07	1.15778E-06
117	2133	11	10991.75	-8858.337	8858.34	5826.436601	2.94574E-08	3.24031E-07	3.56434E-06
110	3049	0.25	9943.71	-6895.109	6895.11	5481.359438	3.32831E-08	8.32077E-09	2.08015E-09
109	856	1.1	10026.58	-9170.877	9170.88	5598.644607	3.25542E-08	3.58246E-08	3.98748E-08
101	2058	0.085	9927.62	-7870.029	7870.03	5476.062903	3.33475E-08	2.83454E-09	2.40936E-10
102	2678	0.13	9932.01	-7253.993	7253.99	5477.597412	3.33299E-08	4.33289E-09	5.63275E-10
D1-1A	8114	2.29	10142.59	-2028.593	2028.59	5546.843847	3.25019E-08	7.44292E-08	1.70443E-07
D1-1B	8944	5.12	10418.50	-1474.996	1475.00	5637.687417	3.14628E-08	1.6109E-07	8.2478E-07
D1-2A	6945	1.37	10052.90	-3108.000	3108.00	5517.311662	3.28507E-08	4.50065E-08	6.16675E-08
D1-2B	6285	2.29	10142.59	-3857.193	3857.15	5546.843847	3.25019E-08	7.44292E-08	1.70443E-07
D2-1A	10471	3.03	10214.74	255.863	255.86	5570.597996	3.22523E-08	9.76425E-08	2.95857E-07
D2-1B	8782	3.22	10233.26	-1451.161	1451.16	5576.637034	3.21548E-08	1.03538E-07	3.33394E-07
EC-1A	8337	4.49	10357.08	-2019.776	2019.78	5617.46429	3.16898E-08	1.42287E-07	5.38869E-07
EC-1B	7320	4.58	10365.85	-3045.950	3045.95	5620.353308	3.16572E-08	1.4499E-07	6.64054E-07
EC-2A	9803	12.6	11147.74	-1344.738	1344.74	5877.790923	2.89448E-08	3.64705E-07	4.59528E-06
EC-2B	3750	5.67	10472.12	-6711.917	6711.92	5655.342528	3.12867E-08	1.77282E-07	1.00519E-06
EC-3A	9344	24.4	12298.15	-2954.446	2954.45	6256.579299	2.55442E-08	6.23327E-07	1.52092E-05
EC-3B	31228	22.1	12073.91	19154.488	19154.49	6182.748838	2.61599E-08	5.78135E-07	1.27768E-05
EC-4A	26257	28.8	12727.11	13530.088	13530.09	6397.820185	2.44307E-08	7.03604E-07	2.02638E-05
EC-4B	9798	7.66	10666.13	-867.826	867.83	5719.221928	3.05722E-08	2.34183E-07	1.79384E-06
LC-1A	6839	0.721	9989.63	-3150.928	3150.93	5498.478631	3.31002E-08	2.38653E-08	1.72069E-08
LC-1B	15394	0.964	10013.32	5380.482	5380.48	5504.27698	3.30065E-08	3.18182E-08	3.06728E-08
MC-1A	10308	9.35	10830.89	-522.488	522.49	5773.471259	3.00003E-08	2.80503E-07	2.6227E-06
MC-1B	10040	2.86	10198.16	-157.864	157.86	5565.140952	3.22885E-08	9.23451E-08	2.64107E-07
MC-2A	8594	4.98	10404.85	-1810.547	1810.55	5633.133389	3.15131E-08	1.56935E-07	7.81537E-07
MC-2B	9116	14.2	11303.73	-2187.925	2187.93	5929.157245	2.84455E-08	4.03927E-07	5.73576E-06
MC-3A	5033	5.68	10473.09	-5440.192	5440.19	5655.86353	3.12632E-08	1.77575E-07	1.00862E-06
MC-3B	6018	18	11674.20	-5655.896	5655.90	6051.138011	2.73103E-08	4.91585E-07	8.84853E-06
PC-1A	40766	31.1	12951.34	27814.956	27814.96	6471.650648	2.38765E-08	7.42558E-07	2.30935E-05
PC-1B	18361	24.5	12307.90	6052.905	6052.90	6259.789319	2.552E-08	6.2524E-07	1.53184E-05
PC-2A	3534	1.24	10040.23	-6506.826	6506.83	5513.138636	3.29005E-08	4.07956E-08	5.05878E-08
PC-2B	3473	1.03	10019.75	-6546.453	6546.45	5506.397593	3.29811E-08	3.39705E-08	3.49896E-08
PC-3A	1691	1.89	10103.60	-8412.596	8412.60	5534.003766	3.26529E-08	6.17139E-08	1.16639E-07
PC-3B	1128	0.604	9978.22	-8850.851	8850.85	5492.722907	3.31455E-08	2.00199E-08	1.2092E-08
						SUM	1.24885E-08	1.28882E-05	0.003945847

OLS Error Variance 282

$$Var = \frac{\sum w_i}{\left(\sum w_i\right)\left(\sum w_i x_i^2\right) - \left(\sum w_i x_i\right)^2}$$

Location	PCDD/F (mg/kg)	Ar1268 (mg/kg)
36	27038	55
61	141906	1300
68	64192	330
1718	18409	56
BR048	2981	1.4
C-15	10834	0.099
C-6	59189	7.58
C-8	10654	2.2
111	9396	6.1
EPA-E3	240328	3800
EPA-F2	94088	1188
EPA-H1	538204	4000
GRID MARSH	5980	6.1
117	2133	11
110	3049	0.25
100	856	1.1
101	2058	0.085
102	2678	0.13
D1-1A	8114	2.29
D1-1B	8944	5.12
D1-2A	6945	1.37
D1-2B	6285	2.29
D2-1A	10471	3.03
D2-1B	8782	3.22
EC-1A	8337	4.49
EC-1B	7320	4.58
EC-2A	9803	12.6
EC-2B	3760	5.67
EC-3A	9344	24.4
EC-3B	31228	22.1
EC-4A	26257	28.8
EC-4B	9798	7.66
LC-1A	6839	0.721
LC-1B	15394	0.964
MC-1A	10308	9.35
MC-1B	10040	2.86
MC-2A	8594	4.98
MC-2B	9116	14.2
MC-3A	5033	5.68
MC-3B	6018	18
PC-1A	40766	31.1
PC-1B	18361	24.5
PC-2A	3534	1.24
PC-2B	3473	1.03
PC-3A	1691	1.89
PC-3B	1128	0.604

Weighted Least Squares performed with "Real Stats" Add-In

$$Pred\ Y_i' = Abs(Res)x + \partial_1$$

$$W_i = \frac{1}{Pred\ Y_i'^2}$$

WLS solution is asymptotic at Iteration #4.

Iteration #1

Location	PCDD/F (mg/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight
36	27038	55	1.55E+04	1.18E+04	1.18E+04	7.24E+03	1.90836E-08
61	141906	1300	1.37E+05	5.25E+03	5.25E+03	4.72E+04	4.48797E-10
68	64192	330	4.21E+04	2.21E+04	2.21E+04	1.61E+04	3.87403E-09
1718	18409	56	1.54E+04	3.03E+03	3.03E+03	7.27E+03	1.89155E-08
BR048	2981	1.4	1.01E+04	-7.07E+03	7.07E+03	5.52E+03	3.28393E-08
C-15	10834	0.099	9.93E+03	9.05E+02	9.05E+02	5.48E+03	3.3342E-08
C-6	59189	7.58	1.07E+04	4.85E+04	4.85E+04	5.72E+03	3.05996E-08
C-8	10654	2.2	1.01E+04	5.21E+02	5.21E+02	5.54E+03	3.25357E-08
111	9396	6.1	1.05E+04	-1.12E+03	1.12E+03	5.67E+03	3.11146E-08
EPA-E3	240328	3800	3.80E+05	-1.40E+05	1.40E+05	1.27E+05	6.15591E-11
EPA-F2	94088	1188	1.26E+05	-3.17E+04	3.17E+04	4.36E+04	5.25848E-10
EPA-H1	538204	4000	4.00E+05	1.38E+05	1.38E+05	1.34E+05	5.57965E-11
GRID MARSH	5980	6.1	1.05E+04	-4.53E+03	4.53E+03	5.67E+03	3.11146E-08
117	2133	11	1.10E+04	-8.86E+03	8.86E+03	5.83E+03	2.94574E-08
110	3049	0.25	9.94E+03	-6.90E+03	6.90E+03	5.48E+03	3.32831E-08
100	856	1.1	1.00E+04	-9.17E+03	9.17E+03	5.51E+03	3.29542E-08
101	2058	0.085	9.93E+03	-7.87E+03	7.87E+03	5.48E+03	3.33475E-08
102	2678	0.13	9.93E+03	-7.25E+03	7.25E+03	5.48E+03	3.33299E-08
D1-1A	8114	2.29	1.01E+04	-2.03E+03	2.03E+03	5.55E+03	3.25019E-08
D1-1B	8944	5.12	1.04E+04	-1.47E+03	1.47E+03	5.64E+03	3.14628E-08
D1-2A	6945	1.37	1.01E+04	-3.11E+03	3.11E+03	5.52E+03	3.28507E-08
D1-2B	6285	2.29	1.01E+04	-3.86E+03	3.86E+03	5.55E+03	3.25019E-08
D2-1A	10471	3.03	1.02E+04	2.56E+02	2.56E+02	5.57E+03	3.22253E-08
D2-1B	8782	3.22	1.02E+04	-1.45E+03	1.45E+03	5.58E+03	3.21548E-08
EC-1A	8337	4.49	1.04E+04	-2.02E+03	2.02E+03	5.62E+03	3.16898E-08
EC-1B	7320	4.58	1.04E+04	-3.05E+03	3.05E+03	5.62E+03	3.16572E-08
EC-2A	9803	12.6	1.11E+04	-1.34E+03	1.34E+03	5.88E+03	2.89448E-08
EC-2B	3760	5.67	1.05E+04	-6.71E+03	6.71E+03	5.66E+03	3.12667E-08
EC-3A	9344	24.4	1.23E+04	-2.95E+03	2.95E+03	6.26E+03	2.55462E-08
EC-3B	31228	22.1	1.21E+04	1.92E+04	1.92E+04	6.18E+03	2.61599E-08
EC-4A	26257	28.8	1.27E+04	1.35E+04	1.35E+04	6.40E+03	2.44307E-08
EC-4B	9798	7.66	1.07E+04	-8.68E+02	8.68E+02	5.72E+03	3.05722E-08
LC-1A	6839	0.721	9.99E+03	-3.15E+03	3.15E+03	5.50E+03	3.31002E-08
LC-1B	15394	0.964	1.00E+04	5.38E+03	5.38E+03	5.50E+03	3.30065E-08
MC-1A	10308	9.35	1.08E+04	-5.22E+02	5.22E+02	5.77E+03	3.00003E-08
MC-1B	10040	2.86	1.02E+04	-1.58E+02	1.58E+02	5.57E+03	3.22885E-08
MC-2A	8594	4.98	1.04E+04	-1.81E+03	1.81E+03	5.63E+03	3.15131E-08
MC-2B	9116	14.2	1.13E+04	-2.19E+03	2.19E+03	5.93E+03	2.84455E-08
MC-3A	5033	5.68	1.05E+04	-5.44E+03	5.44E+03	5.66E+03	3.12632E-08
MC-3B	6018	18	1.17E+04	-5.66E+03	5.66E+03	6.05E+03	2.73103E-08
PC-1A	40766	31.1	1.30E+04	2.78E+04	2.78E+04	6.47E+03	2.38765E-08
PC-1B	18361	24.5	1.23E+04	6.05E+03	6.05E+03	6.26E+03	2.552E-08
PC-2A	3534	1.24	1.00E+04	-6.51E+03	6.51E+03	5.51E+03	3.29005E-08
PC-2B	3473	1.03	1.00E+04	-6.55E+03	6.55E+03	5.51E+03	3.29811E-08
PC-3A	1691	1.89	1.01E+04	-8.41E+03	8.41E+03	5.53E+03	3.26529E-08
PC-3B	1128	0.604	9.98E+03	-8.85E+03	8.85E+03	5.49E+03	3.31455E-08

OVERALL FIT

Multiple R	0.51904768		AIC	52.77318406
R Square	0.26941050		AICc	53.05225383
Adjusted R Square	0.25317517		BSC	54.60182546
Standard Error	1.77554660			
Observations	46			

ANOVA

	df	SS	MS	F	p-value	sig
				Alpha	5.00E-02	
Regression	1	51.1514453	51.15145	16.22534	0.00022	yes
Residual	44	138.7128914	3.15257			
Total	45	189.8643367				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	9370.6689	1616.214331	5.80E+00	6.68E-07	6.11E+03	1.26E+04	
Ar1268 (mg/kg)	115.8194	28.75307607	4.03E+00	2.19E-04	5.79E+01	1.74E+02	1

Iteration #2

Location	PCDD/F (mg/kg)	Ar1268 (mg/kg)	Pred Y2	Residual	ABS(Res)	Pred Y2'	Weight
36	27038	55	1.57E+04	1.13E+04	1.13E+04	7.49E+03	1.78237E-08
61	141906	1300	1.60E+05	-1.80E+04	1.80E+04	4.78E+04	4.38001E-10
68	64192	330	4.76E+04	1.66E+04	1.66E+04	1.64E+04	3.72254E-09
1718	18409	56	1.59E+04	2.55E+03	2.55E+03	7.52E+03	1.76707E-08
BR048	2981	1.4	9.53E+03	-6.55E+03	6.55E+03	5.76E+03	3.01859E-08
C-15	10834	0.099	9.38E+03	1.45E+03	1.45E+03	5.71E+03	3.06324E-08
C-6	59189	7.58	1.02E+04	4.89E+04	4.89E+04	5.96E+03	2.81926E-08
C-8	10654	2.2	9.63E+03	1.03E+03	1.03E+03	5.78E+03	2.99162E-08
111	9396	6.1	1.01E+04	-6.81E+02	6.81E+02	5.91E+03	2.86516E-08
EPA-E3	240328	3800	4.49E+05	-2.09E+05	2.09E+05	1.29E+05	6.03839E-11
EPA-F2	94088	1188	1.47E+05	-5.29E+04	5.29E+04	4.42E+04	5.12858E-10
EPA-H1	538204	4000	4.73E+05	6.56E+04	6.56E+04	1.35E+05	5.47391E-11
GRID MARSH	5980	6.1	1.01E+04	-4.10E+03	4.10E+03	5.91E+03	2.86516E-08
117	2133	11	1.06E+04	-8.51E+03	8.51E+03	6.07E+03	2.71732E-08
110	3049	0.25	9.40E+03	-6.35E+03	6.35E+03	5.72E+03	3.05801E-08
100	856	1.1	9.50E+03	-8.64E+03	8.64E+03	5.75E+03	3.0288E-08
101	2058	0.085	9.38E+03	-7.32E+03	7.32E+03	5.71E+03	3.06373E-08
102	2678	0.13	9.39E+03	-6.71E+03	6.71E+03	5.71E+03	3.06217E-08
D1-1A	8114	2.29	9.64E+03	-1.52E+03	1.52E+03	5.78E+03	2.9886E-08
D1-1B	8944	5.12	9.96E+03	-1.02E+03	1.02E+03	5.88E+03	2.89617E-08
D1-2A	6945	1.37	9.53E+03	-2.58E+03	2.58E+03	5.75E+03	3.01961E-08
D1-2B	6285	2.29	9.64E+03	-3.35E+03	3.35E+03	5.78E+03	2.9886E-08
D2-1A	10471	3.03	9.72E+03	7.49E+02	7.49E+02	5.81E+03	2.96401E-08
D2-1B	8782	3.22	9.74E+03	-9.62E+02	9.62E+02	5.81E+03	2.95774E-08
EC-1A	8337	4.49	9.89E+03	-1.55E+03	1.55E+03	5.86E+03	2.91637E-08
EC-1B	7320	4.58	9.90E+03	-2.58E+03	2.58E+03	5.86E+03	2.91347E-08
EC-2A	9803	12.6	1.08E+04	-1.03E+03	1.03E+03	6.12E+03	2.67152E-08
EC-2B	3760	5.67	1.00E+04	-6.27E+03	6.27E+03	5.89E+03	2.8787E-08
EC-3A	9344	24.4	1.22E+04	-2.85E+03	2.85E+03	6.50E+03	2.36684E-08
EC-3B	31228	22.1	1.19E+04	1.93E+04	1.93E+04	6.43E+03	2.42199E-08
EC-4A	26257	28.8	1.27E+04	1.36E+04	1.36E+04	6.64E+03	2.26645E-08
EC-4B	9798	7.66	1.03E+04	-4.60E+02	4.60E+02	5.96E+03	2.81681E-08
LC-1A	6839	0.721	9.45E+03	-2.62E+03	2.62E+03	5.73E+03	3.04177E-08
LC-1B	15394	0.964	9.48E+03	5.91E+03	5.91E+03	5.74E+03	3.03344E-08
MC-1A	10308	9.35	1.05E+04	-1.45E+02	1.45E+02	6.01E+03	2.7658E-08
MC-1B	10040	2.86	9.70E+03	3.38E+02	3.38E+02	5.80E+03	2.96963E-08
MC-2A	8594	4.98	9.95E+03	-1.35E+03	1.35E+03	5.87E+03	2.90064E-08
MC-2B	9116	14.2	1.10E+04	-1.90E+03	1.90E+03	6.17E+03	2.62687E-08
MC-3A	5033	5.68	1.00E+04	-5.00E+03	5.00E+03	5.89E+03	2.87838E-08
MC-3B	6018	18	1.15E+04	-5.44E+03	5.44E+03	6.29E+03	2.5252E-08
PC-1A	40766	31.1	1.30E+04	2.78E+04	2.78E+04	6.72E+03	2.21649E-08
PC-1B	18361	24.5	1.22E+04	6.15E+03	6.15E+03	6.50E+03	2.36448E-08
PC-2A	3534	1.24	9.51E+03	-5.98E+03	5.98E+03	5.75E+03	3.02403E-08
PC-2B	3473	1.03	9.49E+03	-6.02E+03	6.02E+03	5.74E+03	3.03119E-08
PC-3A	1691	1.89	9.59E+03	-7.90E+03	7.90E+03	5.77E+03	3.00203E-08
PC-3B	1128	0.604	9.44E+03	-8.31E+03	8.31E+03	5.73E+03	3.04579E-08

OVERALL FIT

Multiple R	0.526023839		AIC	49.18547376
R Square	0.276701079		AICc	49.46454353
Adjusted R Square	0.26062777		BSC	51.01411516
Standard Error	1.707638575			
Observations	46			

ANOVA

	df	SS	MS	F	p-value	sig
				Alpha	0.05	
Regression	1	49.0837376	49.08374	16.83238718	0.000174	yes
Residual	44	128.3052981	2.91603			
Total	45	177.3890357				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	9395.084739	1618.654275	5.804226	6.54089E-07	6132.851	12657.22	
Ar1268 (mg/kg)	114.932189	28.0135935	4.102729	0.000173679	58.4745	171.3899	1

Iteration #3

Location	PCDD/F (mg/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight
36	27038	55	1.57E+04	1.13E+04	1.13E+04	7.47E+03	1.79253E-08
61	141906	1300	1.59E+05	-1.69E+04	1.69E+04	4.77E+04	4.39072E-10
68	64192	330	4.73E+04	1.69E+04	1.69E+04	1.64E+04	3.73595E-09
1718	18409	56	1.58E+04	2.58E+03	2.58E+03	7.50E+03	1.77711E-08
BR048	2981	1.4	9.56E+03	-6.57E+03	6.57E+03	5.74E+03	3.03932E-08
C-15	10834	0.099	9.41E+03	1.43E+03	1.43E+03	5.69E+03	3.08439E-08
C-6	59189	7.58	1.03E+04	4.89E+04	4.89E+04	5.94E+03	2.83814E-08
C-8	10654	2.2	9.65E+03	1.01E+03	1.01E+03	5.76E+03	3.01209E-08
111	9396	6.1	1.01E+04	-7.00E+02	7.00E+02	5.89E+03	2.88446E-08
EPA-E3	240328	3800	4.46E+05	-2.06E+05	2.06E+05	1.29E+05	6.05087E-11
EPA-F2	94088	1188	1.46E+05	-5.18E+04	5.18E+04	4.41E+04	5.14138E-10
EPA-H1	538204	4000	4.69E+05	6.91E+04	6.91E+04	1.35E+05	5.48517E-11
GRID MARSH	5980	6.1	1.01E+04	-4.12E+03	4.12E+03	5.89E+03	2.88446E-08
117	2133	11	1.07E+04	-8.53E+03	8.53E+03	6.05E+03	2.73528E-08
110	3049	0.25	9.42E+03	-6.38E+03	6.38E+03	5.70E+03	3.07911E-08
100	856	1.1	9.52E+03	-8.67E+03	8.67E+03	5.73E+03	3.04963E-08
101	2058	0.085	9.40E+03	-7.35E+03	7.35E+03	5.69E+03	3.08488E-08
102	2678	0.13	9.41E+03	-6.73E+03	6.73E+03	5.69E+03	3.08331E-08
D1-1A	8114	2.29	9.66E+03	-1.54E+03	1.54E+03	5.76E+03	3.00905E-08
D1-1B	8944	5.12	9.98E+03	-1.04E+03	1.04E+03	5.86E+03	2.91576E-08
D1-2A	6945	1.37	9.55E+03	-2.61E+03	2.61E+03	5.74E+03	3.04035E-08
D1-2B	6285	2.29	9.66E+03	-3.37E+03	3.37E+03	5.76E+03	3.00905E-08
D2-1A	10471	3.03	9.74E+03	7.27E+02	7.27E+02	5.79E+03	2.98423E-08
D2-1B	8782	3.22	9.77E+03	-9.83E+02	9.83E+02	5.79E+03	2.97791E-08
EC-1A	8337	4.49	9.91E+03	-1.57E+03	1.57E+03	5.84E+03	2.93615E-08
EC-1B	7320	4.58	9.92E+03	-2.60E+03	2.60E+03	5.84E+03	2.93322E-08
EC-2A	9803	12.6	1.08E+04	-1.04E+03	1.04E+03	6.10E+03	2.68907E-08
EC-2B	3760	5.67	1.00E+04	-6.29E+03	6.29E+03	5.87E+03	2.89813E-08
EC-3A	9344	24.4	1.22E+04	-2.86E+03	2.86E+03	6.48E+03	2.38172E-08
EC-3B	31228	22.1	1.19E+04	1.93E+04	1.93E+04	6.41E+03	2.43735E-08
EC-4A	26257	28.8	1.27E+04	1.36E+04	1.36E+04	6.62E+03	2.28049E-08
EC-4B	9798	7.66	1.03E+04	-4.77E+02	4.77E+02	5.94E+03	2.83567E-08
LC-1A	6839	0.721	9.48E+03	-2.64E+03	2.64E+03	5.71E+03	3.06272E-08
LC-1B	15394	0.964	9.51E+03	5.89E+03	5.89E+03	5.72E+03	3.05432E-08
MC-1A	10308	9.35	1.05E+04	-1.61E+02	1.61E+02	5.99E+03	2.7842E-08
MC-1B	10040	2.86	9.72E+03	3.17E+02	3.17E+02	5.78E+03	2.98991E-08
MC-2A	8594	4.98	9.97E+03	-1.37E+03	1.37E+03	5.85E+03	2.92027E-08
MC-2B	9116	14.2	1.10E+04	-1.91E+03	1.91E+03	6.15E+03	2.64402E-08
MC-3A	5033	5.68	1.00E+04	-5.01E+03	5.01E+03	5.87E+03	2.89781E-08
MC-3B	6018	18	1.15E+04	-5.45E+03	5.45E+03	6.27E+03	2.54146E-08
PC-1A	40766	31.1	1.30E+04	2.78E+04	2.78E+04	6.70E+03	2.23012E-08
PC-1B	18361	24.5	1.22E+04	6.15E+03	6.15E+03	6.48E+03	2.37935E-08
PC-2A	3534	1.24	9.54E+03	-6.00E+03	6.00E+03	5.73E+03	3.04481E-08
PC-2B	3473	1.03	9.51E+03	-6.04E+03	6.04E+03	5.72E+03	3.05204E-08
PC-3A	1691	1.89	9.61E+03	-7.92E+03	7.92E+03	5.75E+03	3.0226E-08
PC-3B	1128	0.604	9.46E+03	-8.34E+03	8.34E+03	5.71E+03	3.06678E-08

OVERALL FIT

Multiple R	0.52550658		AIC	49.47918564
R Square	0.27615716		AICc	49.75825541
Adjusted R Square	0.26007177		BSC	51.30782704
Standard Error	1.71309896			
Observations	46			

ANOVA

	df	SS	MS	F	p-value	sig
				Alpha	5.00E-02	
Regression	1	49.26399334	49.26399	16.78668	0.00018	yes
Residual	44	129.1271536	2.93471			
Total	45	178.391147				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	9393.2576	1618.47326	5.80E+00	6.55E-07	6.13E+03	1.27E+04	
Ar1268 (mg/kg)	114.9963	28.0673548	4.10E+00	1.77E-04	5.84E+01	1.72E+02	1

Iteration #4

Location	PCDD/F (mg/kg)	Ar1268 (mg/kg)	Pred Y2	Residual	ABS(Res)	Pred Y2'	Weight
36	27038	55	1.57E+04	1.13E+04	1.13E+04	7.47E+03	1.79E-08
61	141906	1300	1.59E+05	-1.70E+04	1.70E+04	4.77E+04	4.39E-10
68	64192	330	4.73E+04	1.68E+04	1.68E+04	1.64E+04	3.73E-09
1718	18409	56	1.58E+04	2.58E+03	2.58E+03	7.50E+03	1.78E-08
BR048	2981	1.4	9.55E+03	-6.57E+03	6.57E+03	5.74E+03	3.04E-08
C-15	10834	0.099	9.40E+03	1.43E+03	1.43E+03	5.70E+03	3.08E-08
C-6	59189	7.58	1.03E+04	4.89E+04	4.89E+04	5.94E+03	2.84E-08
C-8	10654	2.2	9.65E+03	1.01E+03	1.01E+03	5.76E+03	3.01E-08
111	9396	6.1	1.01E+04	-6.98E+02	6.98E+02	5.89E+03	2.88E-08
EPA-E3	240328	3800	4.46E+05	-2.06E+05	2.06E+05	1.29E+05	6.05E-11
EPA-F2	94088	1188	1.46E+05	-5.19E+04	5.19E+04	4.41E+04	5.14E-10
EPA-H1	538204	4000	4.69E+05	6.88E+04	6.88E+04	1.35E+05	5.48E-11
GRID MARSH	5980	6.1	1.01E+04	-4.11E+03	4.11E+03	5.89E+03	2.88E-08
117	2133	11	1.07E+04	-8.52E+03	8.52E+03	6.05E+03	2.73E-08
110	3049	0.25	9.42E+03	-6.37E+03	6.37E+03	5.70E+03	3.08E-08
100	856	1.1	9.52E+03	-8.66E+03	8.66E+03	5.73E+03	3.05E-08
101	2058	0.085	9.40E+03	-7.35E+03	7.35E+03	5.69E+03	3.08E-08
102	2678	0.13	9.41E+03	-6.73E+03	6.73E+03	5.70E+03	3.08E-08
D1-1A	8114	2.29	9.66E+03	-1.54E+03	1.54E+03	5.77E+03	3.01E-08
D1-1B	8944	5.12	9.98E+03	-1.04E+03	1.04E+03	5.86E+03	2.91E-08
D1-2A	6945	1.37	9.55E+03	-2.61E+03	2.61E+03	5.74E+03	3.04E-08
D1-2B	6285	2.29	9.66E+03	-3.37E+03	3.37E+03	5.77E+03	3.01E-08
D2-1A	10471	3.03	9.74E+03	7.29E+02	7.29E+02	5.79E+03	2.98E-08
D2-1B	8782	3.22	9.76E+03	-9.81E+02	9.81E+02	5.80E+03	2.98E-08
EC-1A	8337	4.49	9.91E+03	-1.57E+03	1.57E+03	5.84E+03	2.93E-08
EC-1B	7320	4.58	9.92E+03	-2.60E+03	2.60E+03	5.84E+03	2.93E-08
EC-2A	9803	12.6	1.08E+04	-1.04E+03	1.04E+03	6.10E+03	2.69E-08
EC-2B	3760	5.67	1.00E+04	-6.29E+03	6.29E+03	5.88E+03	2.90E-08
EC-3A	9344	24.4	1.22E+04	-2.86E+03	2.86E+03	6.48E+03	2.38E-08
EC-3B	31228	22.1	1.19E+04	1.93E+04	1.93E+04	6.41E+03	2.44E-08
EC-4A	26257	28.8	1.27E+04	1.36E+04	1.36E+04	6.62E+03	2.28E-08
EC-4B	9798	7.66	1.03E+04	-4.76E+02	4.76E+02	5.94E+03	2.83E-08
LC-1A	6839	0.721	9.48E+03	-2.64E+03	2.64E+03	5.72E+03	3.06E-08
LC-1B	15394	0.964	9.50E+03	5.89E+03	5.89E+03	5.72E+03	3.05E-08
MC-1A	10308	9.35	1.05E+04	-1.60E+02	1.60E+02	5.99E+03	2.78E-08
MC-1B	10040	2.86	9.72E+03	3.18E+02	3.18E+02	5.78E+03	2.99E-08
MC-2A	8594	4.98	9.97E+03	-1.37E+03	1.37E+03	5.85E+03	2.92E-08
MC-2B	9116	14.2	1.10E+04	-1.91E+03	1.91E+03	6.15E+03	2.64E-08
MC-3A	5033	5.68	1.00E+04	-5.01E+03	5.01E+03	5.88E+03	2.90E-08
MC-3B	6018	18	1.15E+04	-5.44E+03	5.44E+03	6.27E+03	2.54E-08
PC-1A	40766	31.1	1.30E+04	2.78E+04	2.78E+04	6.70E+03	2.23E-08
PC-1B	18361	24.5	1.22E+04	6.15E+03	6.15E+03	6.48E+03	2.38E-08
PC-2A	3534	1.24	9.54E+03	-6.00E+03	6.00E+03	5.73E+03	3.04E-08
PC-2B	3473	1.03	9.51E+03	-6.04E+03	6.04E+03	5.73E+03	3.05E-08
PC-3A	1691	1.89	9.61E+03	-7.92E+03	7.92E+03	5.75E+03	3.02E-08
PC-3B	1128	0.604	9.46E+03	-8.34E+03	8.34E+03	5.71E+03	3.07E-08

OVERALL FIT

Multiple R	0.525543757		AIC	49.45802902
R Square	0.27619624		AICc	49.73709879
Adjusted R Square	0.260111712		BSC	51.28667042
Standard Error	1.712705053			
Observations	46			

ANOVA

	df	SS	MS	F	p-value	sig
				Alpha	0.05	
Regression	1	49.25096707	49.25097	16.7899578	0.000177	yes
Residual	44	129.0677783	2.933359			
Total	45	178.3187454				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	**9393.385488**	**1618.48627**	5.803809	6.55009E-07	6131.541	12655.23	
Ar1268 (mg/kg)	**114.9916767**	**28.06348515**	4.097555	0.000176506	58.43344	171.5499	1

Case 2a: PCDD/F Concentration and Aroclor 1268 (Cumulative Data Set)

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight	Weight * X	Weight*X^2
36	27038	55	15717.93	11319.972	11319.97	7470.494248	1.79185E-08	9.85517E-07	5.42034E-05
61	141906	1300	158882.57	-16976.567	16976.57	47727.38638	4.39E-10	5.707E-07	0.00074191
68	64192	330	47340.64	16851.360	16851.36	16362.57886	3.73505E-09	1.23257E-06	0.000406747
1718	18409	56	15832.92	2576.281	2576.28	7502.829101	1.77644E-08	9.94805E-07	5.57091E-05
BR048	2981	1.4	9554.37	-6573.374	6573.37	5737.34612	3.03793E-08	4.2531E-08	5.95434E-08
C-15	10834	0.099	9404.77	1429.230	1429.23	5695.278477	3.08298E-08	3.05215E-09	3.02162E-10
C-6	59189	7.58	10265.02	48923.977	48923.98	5937.175513	2.83688E-08	2.15035E-07	1.62997E-06
C-8	10654	2.2	9646.37	1008.033	1008.03	5763.214003	3.01072E-08	6.62359E-08	1.45719E-07
111	9396	6.1	10094.83	-698.468	698.47	5889.31993	2.88317E-08	1.75873E-07	1.07283E-06
EPA-E3	240328	3800	446361.76	-206033.557	206033.56	128564.5192	6.05003E-11	2.29901E-07	0.000873625
EPA-F2	94088	1188	146003.50	-51915.797	51915.80	44105.88283	5.14052E-10	6.10694E-07	0.000725504
EPA-H1	538204	4000	469360.09	68844.108	68844.11	135031.4898	5.48441E-11	2.19376E-07	0.000877506
GRID MARSH	5980	6.1	10094.83	-4114.835	4114.83	5889.31993	2.88317E-08	1.75873E-07	1.07283E-06
117	2133	11	10658.29	-8524.880	8524.88	6047.76071	2.73408E-08	3.00749E-07	3.30823E-06
110	3049	0.25	9422.13	-6373.533	6373.53	5700.161039	3.0777E-08	7.69424E-09	1.92356E-09
100	856	1.1	9519.88	-8664.176	8664.18	5727.645665	3.04823E-08	3.35305E-08	3.68836E-08
101	2058	0.085	9403.16	-7345.566	7345.57	5694.825789	3.08347E-08	2.62095E-09	2.2278E-10
102	2678	0.13	9408.33	-6730.317	6730.32	5696.280857	3.08189E-08	4.00646E-09	5.2084E-10
D1-1A	8114	2.29	9656.72	-1542.716	1542.72	5766.12414	3.00768E-08	6.88759E-08	1.57726E-07
D1-1B	8944	5.12	9982.14	-1038.643	1038.64	5857.631774	2.91445E-08	1.4922E-07	7.64004E-07
D1-2A	6945	1.37	9550.92	-2606.024	2606.02	5736.376075	3.03896E-08	4.16337E-08	5.70382E-08
D1-2B	6285	2.29	9656.72	-3371.316	3371.32	5766.12414	3.00768E-08	6.88759E-08	1.57726E-07
D2-1A	10471	3.03	9741.81	728.790	728.79	5790.051931	2.98288E-08	9.03811E-08	2.73855E-07
D2-1B	8782	3.22	9763.66	-981.559	981.56	5796.195553	2.97656E-08	9.58451E-08	3.08621E-07
EC-1A	8337	4.49	9909.70	-1572.398	1572.40	5837.260817	2.93482E-08	1.31774E-07	5.91663E-07
EC-1B	7320	4.58	9920.05	-2600.147	2600.15	5840.170953	2.9319E-08	1.34281E-07	6.15007E-07
EC-2A	9803	12.6	10842.28	-1039.281	1039.28	6099.496475	2.68789E-08	3.38675E-07	4.2673E-06
EC-2B	3760	5.67	10045.39	-6285.188	6285.19	5875.415943	2.89683E-08	1.6425E-07	9.31298E-07
EC-3A	9344	24.4	12199.18	-2855.482	2855.48	6481.047742	2.38073E-08	5.80897E-07	1.41739E-05
EC-3B	31228	22.1	11934.70	19293.698	19293.70	6406.67758	2.43632E-08	5.38427E-07	1.18992E-05
EC-4A	26257	28.8	12705.15	13552.054	13552.05	6623.321096	2.27955E-08	6.56509E-07	1.89075E-05
EC-4B	9798	7.66	10274.22	-475.922	475.92	5939.762301	2.8344E-08	2.17115E-07	1.6631E-06
LC-1A	6839	0.721	9476.29	-2637.594	2637.59	5715.390755	3.06132E-08	2.20721E-08	1.5914E-08
LC-1B	15394	0.964	9504.24	5889.563	5889.56	5723.248125	3.05292E-08	2.94301E-08	2.83706E-08
MC-1A	10308	9.35	10468.56	-160.158	160.16	5994.408203	2.78296E-08	2.60207E-07	2.43294E-06
MC-1B	10040	2.86	9722.26	318.038	318.04	5784.555006	2.98855E-08	8.54724E-08	2.44451E-07
MC-2A	8594	4.98	9966.04	-1371.744	1371.74	5853.104895	2.91895E-08	1.45364E-07	7.23912E-07
MC-2B	9116	14.2	11026.27	-1910.467	1910.47	6151.23224	2.64287E-08	3.75287E-07	5.32908E-06
MC-3A	5033	5.68	10046.54	-5013.638	5013.64	5875.739292	2.89651E-08	1.64522E-07	9.34483E-07
MC-3B	6018	18	11463.24	-5444.936	5444.94	6274.104682	2.54037E-08	4.57266E-07	8.23079E-06
PC-1A	40766	31.1	12969.63	27796.673	27796.67	6697.691258	2.2292E-08	6.93282E-07	2.15611E-05
PC-1B	18361	24.5	12210.68	6150.118	6150.12	6484.281228	2.37835E-08	5.82696E-07	1.42761E-05
PC-2A	3534	1.24	9535.98	-6001.575	6001.58	5732.172544	3.04342E-08	3.77384E-08	4.67956E-08
PC-2B	3473	1.03	9511.83	-6038.527	6038.53	5725.382225	3.05064E-08	3.14216E-08	3.23642E-08
PC-3A	1691	1.89	9610.72	-7919.720	7919.72	5753.190198	3.02122E-08	5.71011E-08	1.07921E-07
PC-3B	1128	0.604	9462.84	-8335.270	8335.27	5711.607577	3.06537E-08	1.85149E-08	1.1183E-08
						SUM	1.15792E-06	1.21079E-05	0.003851276

WLS Error Variance **268**

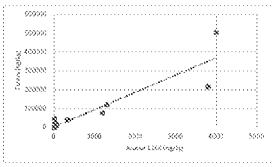
$$Var = \frac{\sum w_i}{\left((\sum w_i)(\sum w_i x_i^2) - (\sum w_i x_i)^2\right)}$$

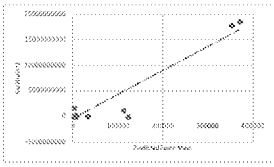
WLS Var:OLS Var = **1.02**

Heteroscedasticity not severe

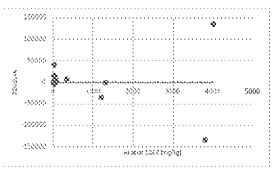
Case 2b: Furan Congener Concentration and Aroclor 1268 (Cumulative Data Set)

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred PCDD/F (ng/kg)	Pred PCDD/F^2	Residual PCDD/F	Residual^2
36	14468	55	7883.67	62152281.15	6584.33	43353376.72
61	122400	1300	122567.26	15022733544.51	-167.26	27976.74
68	40850	330	33215.39	1103262024.10	7634.61	58287280.48
1718	8750	56	7975.79	63613180.49	774.21	599406.61
BR04S	391	1.4	2946.29	8680624.54	-2555.29	6529506.78
C-15	1348	0.099	2826.45	7988807.81	-1478.45	2185808.22
C-6	44710	7.58	3515.56	12359181.23	41194.44	1696981628.31
C-8	2826	2.2	3019.98	9120292.65	-193.98	37629.11
111	5036	6.1	3379.23	11419209.09	1656.85	2745148.52
EPA-E3	219200	3800	352855.59	124507069963.06	-133655.59	17863817711.27
EPA-F2	77700	1188	112250.34	12600139732.47	-34550.34	1193728271.88
EPA-H1	507600	4000	371278.66	137847843539.86	136321.34	18583507877.62
GRID MARSH	3690	6.1	3379.23	11419209.09	310.77	96576.69
117	148	11	3830.60	14673474.58	-3682.99	13564409.13
119	630	0.25	2840.36	8067629.75	-2210.36	4885679.52
109	71	1.1	2918.66	8518549.12	-2848.16	8111988.96
101	161	0.085	2825.16	7981519.41	-2664.06	7097211.95
102	147	0.13	2829.30	8004958.23	-2681.95	7192863.79
D1-1A	1206	2.29	3028.27	9170434.99	-1822.27	3320677.46
D1-1B	1641	5.12	3288.96	10817251.30	-1647.96	2715768.86
D1-2A	565	1.37	2943.53	8664348.25	-2379.03	5659767.09
D1-2B	690	2.29	3028.27	9170434.99	-2427.87	5894565.40
D2-1A	3831	3.03	3096.44	9587528.00	734.56	539581.49
D2-1B	3162	3.22	3113.94	9696621.50	48.06	2309.78
EC-1A	999	4.49	3230.93	10438885.01	-2231.73	4980602.48
EC-1B	1002	4.58	3239.22	10492524.96	-2237.52	5006481.07
EC-2A	2030	12.6	3977.98	15824338.33	-1947.98	3794632.66
EC-2B	230	5.67	3339.62	11153077.99	-3109.72	9670373.61
EC-3A	3810	24.4	5064.94	25653643.73	-1254.94	1574880.98
EC-3B	20737	22.1	4853.08	23552359.79	15883.92	252298996.86
EC-4A	17065	28.8	5470.25	29923635.98	11594.75	134438225.62
EC-4B	3446	7.66	3522.93	12411048.49	-76.93	5918.52
LC-1A	728	0.721	2883.74	8315977.44	-2155.54	4646308.43
LC-1B	2958	0.964	2906.13	8445578.07	51.87	2699.74
MC-1A	2089	9.35	3678.61	13592148.42	-1589.61	2526849.96
MC-1B	1409	2.86	3080.78	9491195.23	-1671.78	2794842.84
MC-2A	1515	4.98	3276.06	10732567.82	-1761.06	3101342.37
MC-2B	2089	14.2	4125.37	17018646.47	-2036.37	4146787.39
MC-3A	1358	5.68	3340.54	11159231.45	-1982.54	3930479.07
MC-3B	1872	18	4475.40	20029245.33	-2603.40	6777714.93
PC-1A	13310	31.1	5682.12	32286434.84	7627.88	58184624.24
PC-1B	4611	24.5	5074.15	25747040.36	-463.15	214511.77
PC-2A	649	1.24	2931.55	8593994.24	-2282.25	5206871.95
PC-2B	207	1.03	2912.21	8480951.29	-2705.51	7319769.59
PC-3A	316	1.89	2991.43	8948632.35	-2675.23	7156836.09
PC-3B	206	0.604	2872.97	8253934.53	-2666.77	7111841.73





Test for Zero Conditional Mean of Errors:



No discernable relationship between residuals and independent variable
$Cov(\hat{u}_i, x_i) = 0$

Tests for Homoscedasticity

BREUSCH-PAGAN SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.956120197
R Square	0.91416583
Adjusted R Square	0.912215054
Standard Error	1112123936
Observations	46

$$\hat{u}^2 = d_0 + x d_1$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p<0.05
Status: Heteroscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	5.79594E+20	5.79594E+20	466.6163645	4.33387E-25
Residual	44	5.44291E+19	1.23682E+18		
Total	45	6.34014E+20			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-164130657.5	170795174	-0.960980651	0.34181337	-508345913	180084198.1	-508345913	180084198.1
Ar1268 (mg/kg)	4322137.276	199559.432	21.6475487	4.33387E-25	3919750.131	4724524.422	3919750.131	4724524.422

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.996001734
R Square	0.992019455
Adjusted R Square	0.991848266
Standard Error	343029509.3
Observations	46

$$\hat{u}^2 = d_0 + \hat{Y} \times d_1 + \hat{Y}^2 \times d_2$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p<0.05
Status: Heteroscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	2	6.28854E+20	3.14477E+20	2672.551431	7.82889E-45
Residual	43	5.05578E+18	1.17669E+17		
Total	45	6.34014E+20			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	11823348.5	5698527.53	2.075854806	0.043521297	339698.773	233097266.3	339698.773	233097266.3
Pred PCDD/F (ng/kg)	-16368.75449	3161.81607	-5.177337831	5.65320E-06	-22744.76905	-9992.748022	-22744.76905	-9992.748022
Pred PCDD/F^2	0.18278571	0.00882452	20.48125232	8.37324E-24	0.164787699	0.20078372	0.164787699	0.20078372

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y	Weight	Weight * X	Weight*X^2
36	14468	55	7883.67	6584.328	6584.33	4144.211888	5.82259E-08	3.20242E-06	0.000176133
61	122400	1300	122567.26	-167.262	167.26	43815.13289	5.20897E-10	6.77166E-07	0.000880316
68	40850	330	33215.39	7634.611	7634.61	12906.86512	6.00288E-09	1.98094E-06	0.000653712
1718	8750	56	7975.79	774.213	774.21	4176.076982	5.73407E-08	3.21108E-06	0.000179821
BR04S	391	1.4	2946.29	-2555.290	2555.29	2436.291113	1.68477E-07	2.35888E-07	3.30216E-07
C-15	1348	0.099	2826.45	-1478.448	1478.45	2394.835797	1.74361E-07	1.72617E-08	1.70891E-09
C-6	44710	7.58	3515.56	41194.437	41194.44	2633.211829	1.44221E-07	1.09319E-06	8.28642E-06
C-8	2826	2.2	3019.98	-193.982	193.98	2461.782467	1.65006E-07	3.63014E-07	7.98631E-07
111	5036	6.1	3379.23	1656.849	1656.85	2586.052822	1.49529E-07	9.12126E-07	5.56397E-06
EPA-E3	219200	3800	352855.59	-133655.594	133655.59	123475.6168	6.559E-11	2.49242E-07	0.0009471.2
EPA-F2	77700	1188	112250.34	-34550.344	34550.34	40246.34321	6.17372E-10	7.33438E-07	0.000871325
EPA-H1	507600	4000	371278.66	136321.349	136321.34	129848.4556	5.93098E-11	2.37239E-07	0.000948957
GRID MARSH	3690	6.1	3379.23	310.768	310.77	2586.052822	1.49529E-07	9.12126E-07	5.56397E-06
117	148	11	3830.60	-3682.989	3682.99	2742.187371	1.32988E-07	1.46285E-06	1.60913E-05
119	630	0.25	2840.36	-2210.357	2210.36	2399.84729	1.73662E-07	4.34155E-08	1.08539E-08
109	71	1.1	2918.66	-2848.155	2848.16	2426.731854	1.69807E-07	1.86788E-07	2.05467E-07
101	161	0.085	2825.16	-2664.059	2664.06	2394.389898	1.74428E-07	1.48262E-08	1.26023E-09
102	147	0.13	2829.30	-2681.951	2681.95	2395.623587	1.74217E-07	2.26482E-08	2.94427E-09
D1-1A	1206	2.29	3028.27	-1822.273	1822.27	2454.650245	1.64623E-07	3.76986E-07	8.63297E-07
D1-1B	1641	5.12	3288.96	-1647.959	1647.96	2554.825913	1.53207E-07	7.84418E-07	4.01622E-06
D1-2A	565	1.37	2943.53	-2379.027	2379.03	2435.335187	1.8861E-07	2.30935E-07	3.16464E-07
D1-2B	690	2.29	3028.27	-2427.873	2427.87	2454.650245	1.64623E-07	3.76986E-07	8.63297E-07
D2-1A	3831	3.03	3096.44	734.562	734.56	2498.229748	1.61517E-07	4.88397E-07	1.48287E-06
D2-1B	3162	3.22	3113.94	48.060	48.06	2494.283945	1.60734E-07	5.17564E-07	1.66656E-06
EC-1A	999	4.49	3230.93	-2231.726	2231.73	2534.751471	1.55843E-07	6.98836E-07	3.13778E-06
EC-1B	1002	4.58	3239.22	-2237.517	2237.52	2537.619248	1.55291E-07	7.11234E-07	3.25745E-06
EC-2A	2030	12.6	3977.98	-1947.982	1947.98	2793.170081	1.28178E-07	1.61501E-06	2.03492E-05
EC-2B	230	5.67	3339.62	-3109.722	3109.72	2572.351219	1.51128E-07	8.58885E-07	4.85854E-06
EC-3A	3810	24.4	5064.94	-1254.943	1254.94	3169.167565	9.95657E-08	2.4294E-06	5.92774E-05
EC-3B	20737	22.1	4853.08	15883.923	15883.92	3095.879292	1.04335E-07	2.30581E-06	5.09585E-05
EC-4A	17065	28.8	5470.25	11594.750	11594.75	3306.370017	9.13081E-08	2.52967E-06	7.57345E-05
EC-4B	3446	7.66	3522.93	-76.932	76.93	2635.780964	1.43942E-07	1.1025E-06	8.44589E-06
LC-1A	728	0.721	2883.74	-2155.544	2155.54	2414.655325	1.7151E-07	1.23659E-07	8.9158E-08
LC-1B	2958	0.964	2906.13	51.872	51.87	2422.398324	1.70415E-07	1.6428E-07	1.58366E-07
MC-1A	2089	9.35	3678.61	-1589.607	1589.61	2689.611451	1.38236E-07	1.29251E-06	1.20849E-05
MC-1B	1409	2.86	3080.78	-1671.778	1671.78	2482.812835	1.62223E-07	4.63957E-07	1.32692E-06
MC-2A	1515	4.98	3276.06	-1761.063	1761.06	2550.384626	1.53743E-07	7.6564E-07	3.81289E-06
MC-2B	2089	14.2	4125.37	-2036.366	2036.37	2844.15279	1.23622E-07	1.75543E-06	2.4927E-05
MC-3A	1358	5.68	3340.54	-1982.544	1982.54	2572.669851	1.51069E-07	8.58184E-07	4.87448E-06
MC-3B	1872	18	4475.40	-2603.404	2603.40	2965.236726	1.13732E-07	2.04717E-06	3.6849E-05
PC-1A	13310	31.1	5682.12	7627.885	7627.88	3382.657662	8.73945E-08	2.71797E-06	8.45288E-05
PC-1B	4611	24.5	5074.15	-463.154	463.15	3172.353984	9.93558E-08	2.43446E-05	5.96443E-05
PC-2A	649	1.24	2931.55	-2282.252	2282.25	2431.192842	1.69185E-07	2.09789E-07	2.60138E-07
PC-2B	207	1.03	2912.21	-2705.507	2705.51	2424.501361	1.7012E-07	1.75224E-07	1.8048E-07
PC-3A	316	1.89	2991.43	-2675.226	2675.23	2451.904567	1.66339E-07	3.1438E-07	5.94178E-07
PC-3B	206	0.604	2872.97	-2666.766	2666.77	2410.927214	1.72041E-07	1.03913E-07	6.27633E-08
						SUM	5.95977E-06	4.4108E-05	0.00515886

OLS Error Variance **207**

$$Var = \frac{\sum w_i}{\left(\left(\sum w_i\right)\left(\sum w_i x_i^2\right) - \left(\sum w_i x_i\right)^2\right)}$$

Location	Furans (ng/kg)	Ar1268 (mg/kg)
36	14468	55
61	122400	1300
68	40850	330
1718	8750	56
BR048	391	1.4
C-15	1348	0.099
C-6	44710	7.58
C-8	2826	2.2
111	5036	6.1
EPA-E3	219200	3800
EPA-F2	77700	1188
EPA-H1	507600	4000
GRID MARSH	3690	6.1
117	148	11
110	630	0.25
100	71	1.1
101	161	0.085
102	147	0.13
D1-1A	1206	2.29
D1-1B	1641	5.12
D1-2A	565	1.37
D1-2B	600	2.29
D2-1A	3831	3.03
D2-1B	3162	3.22
EC-1A	999	4.49
EC-1B	1002	4.58
EC-2A	2030	12.6
EC-2B	230	5.67
EC-3A	3810	24.4
EC-3B	20737	22.1
EC-4A	17065	28.8
EC-4B	3446	7.66
LC-1A	728	0.721
LC-1B	2958	0.964
MC-1A	2089	9.35
MC-1B	1409	2.86
MC-2A	1515	4.98
MC-2B	2089	14.2
MC-3A	1358	5.68
MC-3B	1872	18
PC-1A	13310	31.1
PC-1B	4611	24.5
PC-2A	649	1.24
PC-2B	207	1.03
PC-3A	316	1.89
PC-3B	206	0.604

Weighted Least Squares performed with "Real Stats" Add-In

$$Pred\ Y_i' = Abs(Res)x + \partial_1$$

$$W_i = \frac{1}{Pred\ Y_i'^2}$$

WLS solution is asymptotic at Iteration #4.

Iteration #1

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y	Weight
36	14468	55	7.88E+03	6.58E+03	6.58E+03	4.14E+03	5.82259E-08
61	122400	1300	1.23E+05	-1.67E+02	1.67E+02	4.38E+04	5.20897E-10
68	40850	330	3.52E+04	7.63E+03	7.63E+03	1.29E+04	6.00286E-09
1718	8750	56	7.98E+03	7.74E+02	7.74E+02	4.18E+03	5.73407E-08
BR048	391	1.4	2.95E+03	-2.56E+03	2.56E+03	2.44E+03	1.68477E-07
C-15	1348	0.099	2.83E+03	-1.48E+03	1.48E+03	2.39E+03	1.74361E-07
C-6	44710	7.58	3.52E+03	4.12E+04	4.12E+04	2.63E+03	1.44221E-07
C-8	2826	2.2	3.02E+03	-1.94E+02	1.94E+02	2.46E+03	1.65006E-07
111	5036	6.1	3.38E+03	1.66E+03	1.66E+03	2.59E+03	1.49529E-07
EPA-E3	219200	3800	3.53E+05	-1.34E+05	1.34E+05	1.23E+05	6.559E-11
EPA-F2	77700	1188	1.12E+05	-3.46E+04	3.46E+04	4.02E+04	6.17372E-10
EPA-H1	507600	4000	3.71E+05	1.36E+05	1.36E+05	1.30E+05	5.93098E-11
GRID MARSH	3690	6.1	3.38E+03	3.11E+02	3.11E+02	2.59E+03	1.49529E-07
117	148	11	3.83E+03	-3.68E+03	3.68E+03	2.74E+03	1.32986E-07
110	630	0.25	2.84E+03	-2.21E+03	2.21E+03	2.40E+03	1.73662E-07
100	71	1.1	2.92E+03	-2.85E+03	2.85E+03	2.43E+03	1.69807E-07
101	161	0.085	2.83E+03	-2.66E+03	2.66E+03	2.39E+03	1.74426E-07
102	147	0.13	2.83E+03	-2.68E+03	2.68E+03	2.40E+03	1.74217E-07
D1-1A	1206	2.29	3.03E+03	-1.82E+03	1.82E+03	2.46E+03	1.64623E-07
D1-1B	1641	5.12	3.29E+03	-1.65E+03	1.65E+03	2.55E+03	1.53207E-07
D1-2A	565	1.37	2.94E+03	-2.38E+03	2.38E+03	2.44E+03	1.6861E-07
D1-2B	600	2.29	3.03E+03	-2.43E+03	2.43E+03	2.46E+03	1.64623E-07
D2-1A	3831	3.03	3.10E+03	7.35E+02	7.35E+02	2.49E+03	1.61517E-07
D2-1B	3162	3.22	3.11E+03	4.81E+01	4.81E+01	2.49E+03	1.60734E-07
EC-1A	999	4.49	3.23E+03	-2.23E+03	2.23E+03	2.53E+03	1.55643E-07
EC-1B	1002	4.58	3.24E+03	-2.24E+03	2.24E+03	2.54E+03	1.55291E-07
EC-2A	2030	12.6	3.98E+03	-1.95E+03	1.95E+03	2.79E+03	1.28176E-07
EC-2B	230	5.67	3.34E+03	-3.11E+03	3.11E+03	2.57E+03	1.51126E-07
EC-3A	3810	24.4	5.06E+03	-1.25E+03	1.25E+03	3.17E+03	9.95657E-08
EC-3B	20737	22.1	4.85E+03	1.59E+04	1.59E+04	3.10E+03	1.04335E-07
EC-4A	17065	28.8	5.47E+03	1.16E+04	1.16E+04	3.31E+03	9.13081E-08
EC-4B	3446	7.66	3.52E+03	-7.69E+01	7.69E+01	2.64E+03	1.43942E-07
LC-1A	728	0.721	2.88E+03	-2.16E+03	2.16E+03	2.41E+03	1.7151E-07
LC-1B	2958	0.964	2.91E+03	5.19E+01	5.19E+01	2.42E+03	1.70415E-07
MC-1A	2089	9.35	3.68E+03	-1.59E+03	1.59E+03	2.69E+03	1.38236E-07
MC-1B	1409	2.86	3.08E+03	-1.67E+03	1.67E+03	2.48E+03	1.62223E-07
MC-2A	1515	4.98	3.28E+03	-1.76E+03	1.76E+03	2.55E+03	1.53743E-07
MC-2B	2089	14.2	4.13E+03	-2.04E+03	2.04E+03	2.84E+03	1.23622E-07
MC-3A	1358	5.68	3.34E+03	-1.98E+03	1.98E+03	2.57E+03	1.51089E-07
MC-3B	1872	18	4.48E+03	-2.60E+03	2.60E+03	2.97E+03	1.13732E-07
PC-1A	13310	31.1	5.68E+03	7.63E+03	7.63E+03	3.38E+03	8.73945E-08
PC-1B	4611	24.5	5.07E+03	-4.63E+02	4.63E+02	3.17E+03	9.93658E-08
PC-2A	649	1.24	2.93E+03	-2.28E+03	2.28E+03	2.43E+03	1.69185E-07
PC-2B	207	1.03	2.91E+03	-2.71E+03	2.71E+03	2.42E+03	1.7012E-07
PC-3A	316	1.89	2.99E+03	-2.68E+03	2.68E+03	2.45E+03	1.66339E-07
PC-3B	206	0.604	2.87E+03	-2.67E+03	2.67E+03	2.41E+03	1.72041E-07

OVERALL FIT

Multiple R	0.40557241	AIC	90.60140782
R Square	0.16448898	AICc	90.88047759
Adjusted R Square	0.14592207	BSC	92.43004922
Standard Error	2.67857426		
Observations	46		

ANOVA — Alpha 5.00E-02

	df	*SS*	*MS*	*F*	*p-value*	*sig*
Regression	1	62.15050804	62.15051	8.66238	0.00517	yes
Residual	44	315.6894439	7.17476			
Total	45	377.8399519				

	coeff	*std err*	*t stat*	*p-value*	*lower*	*upper*	*vif*
Intercept	2746.2476	1134.577059	2.42E+00	1.97E-02	4.60E+02	5.03E+03	
Ar1268 (mg/kg)	113.4128	38.53395556	2.94E+00	5.17E-03	3.58E+01	1.91E+02	1

Iteration #2

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred Y2	Residual	ABS(Res)	Pred Y2	Weight
36	14468	55	8.98E+03	5.48E+03	5.48E+03	4.89E+03	4.18277E-08
61	122400	1300	1.50E+05	-2.78E+04	2.78E+04	4.54E+04	4.8534E-10
68	40850	330	4.02E+04	6.78E+02	6.78E+02	1.38E+04	5.22385E-09
1718	8750	56	9.10E+03	-3.47E+02	3.47E+02	4.92E+03	4.12767E-08
BR048	391	1.4	2.91E+03	-2.51E+03	2.51E+03	3.15E+03	1.01049E-07
C-15	1348	0.099	2.76E+03	-1.41E+03	1.41E+03	3.10E+03	1.03823E-07
C-6	44710	7.58	3.61E+03	4.11E+04	4.11E+04	3.35E+03	8.92732E-08
C-8	2826	2.2	3.00E+03	-1.70E+02	1.70E+02	3.17E+03	9.93971E-08
111	5036	6.1	3.44E+03	1.60E+03	1.60E+03	3.30E+03	9.18982E-08
EPA-E3	219200	3800	4.34E+05	-2.15E+05	2.15E+05	1.27E+05	6.22729E-11
EPA-F2	77700	1188	1.37E+05	-5.98E+04	5.98E+04	4.17E+04	5.73753E-10
EPA-H1	507600	4000	4.56E+05	5.12E+04	5.12E+04	1.33E+05	5.63391E-11
GRID MARSH	3690	6.1	3.44E+03	2.52E+02	2.52E+02	3.30E+03	9.18982E-08
117	148	11	3.99E+03	-3.85E+03	3.85E+03	3.46E+03	8.36212E-08
110	630	0.25	2.77E+03	-2.14E+03	2.14E+03	3.11E+03	1.03496E-07
100	71	1.1	2.87E+03	-2.80E+03	2.80E+03	3.14E+03	1.01678E-07
101	161	0.085	2.76E+03	-2.59E+03	2.59E+03	3.10E+03	1.03854E-07
102	147	0.13	2.76E+03	-2.61E+03	2.61E+03	3.10E+03	1.03756E-07
D1-1A	1206	2.29	3.01E+03	-1.80E+03	1.80E+03	3.17E+03	9.92139E-08
D1-1B	1641	5.12	3.33E+03	-1.69E+03	1.69E+03	3.27E+03	9.37006E-08
D1-2A	565	1.37	2.90E+03	-2.34E+03	2.34E+03	3.14E+03	1.01111E-07
D1-2B	600	2.29	3.01E+03	-2.41E+03	2.41E+03	3.17E+03	9.92139E-08
D2-1A	3831	3.03	3.09E+03	7.41E+02	7.41E+02	3.20E+03	9.77262E-08
D2-1B	3162	3.22	3.11E+03	5.06E+01	5.06E+01	3.21E+03	9.73496E-08
EC-1A	999	4.49	3.26E+03	-2.26E+03	2.26E+03	3.25E+03	9.48875E-08
EC-1B	1002	4.58	3.27E+03	-2.26E+03	2.26E+03	3.25E+03	9.47166E-08
EC-2A	2030	12.6	4.18E+03	-2.15E+03	2.15E+03	3.51E+03	8.11596E-08
EC-2B	230	5.67	3.39E+03	-3.16E+03	3.16E+03	3.28E+03	9.26826E-08
EC-3A	3810	24.4	5.51E+03	-1.70E+03	1.70E+03	3.89E+03	6.59469E-08
EC-3B	20737	22.1	5.25E+03	1.55E+04	1.55E+04	3.82E+03	6.85562E-08
EC-4A	17065	28.8	6.01E+03	1.11E+04	1.11E+04	4.04E+03	6.13535E-08
EC-4B	3446	7.66	3.61E+03	-1.69E+02	1.69E+02	3.35E+03	8.91345E-08
LC-1A	728	0.721	2.83E+03	-2.10E+03	2.10E+03	3.12E+03	1.02483E-07
LC-1B	2958	0.964	2.86E+03	1.02E+02	1.02E+02	3.13E+03	1.01966E-07
MC-1A	2089	9.35	3.81E+03	-1.72E+03	1.72E+03	3.40E+03	8.62789E-08
MC-1B	1409	2.86	3.07E+03	-1.66E+03	1.66E+03	3.19E+03	9.8065E-08
MC-2A	1515	4.98	3.31E+03	-1.80E+03	1.80E+03	3.26E+03	9.39624E-08
MC-2B	2089	14.2	4.36E+03	-2.27E+03	2.27E+03	3.56E+03	7.88051E-08
MC-3A	1358	5.68	3.39E+03	-2.03E+03	2.03E+03	3.29E+03	9.26643E-08
MC-3B	1872	18	4.79E+03	-2.92E+03	2.92E+03	3.69E+03	7.36076E-08
PC-1A	13310	31.1	6.27E+03	7.04E+03	7.04E+03	4.11E+03	5.9141E-08
PC-1B	4611	24.5	5.52E+03	-9.14E+02	9.14E+02	3.90E+03	6.58368E-08
PC-2A	649	1.24	2.89E+03	-2.24E+03	2.24E+03	3.14E+03	1.01384E-07
PC-2B	207	1.03	2.86E+03	-2.66E+03	2.66E+03	3.13E+03	1.01826E-07
PC-3A	316	1.89	2.96E+03	-2.64E+03	2.64E+03	3.16E+03	1.00032E-07
PC-3B	206	0.604	2.81E+03	-2.61E+03	2.61E+03	3.12E+03	1.02733E-07

OVERALL FIT

Multiple R	0.445898779	AIC	69.32480105
R Square	0.198825721	AICc	69.60387082
Adjusted R Square	0.181021848	BSC	71.15344245
Standard Error	2.125521528		
Observations	46		

ANOVA — Alpha 0.05

	df	*SS*	*MS*	*F*	*p-value*	*sig*
Regression	1	49.33206111	49.33206	10.91938666	0.001898	yes
Residual	44	198.7850376	4.517842			
Total	45	248.1170988				

	coeff	*std err*	*t stat*	*p-value*	*lower*	*upper*	*vif*
Intercept	2871.6336	1141.544608	2.515568	0.015609032	571.0016	5172.266	
Ar1268 (mg/kg)	106.5762163	32.25233599	3.30445	0.001898034	41.5759	171.5765	1

Iteration #3

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y	Weight
36	14468	55	8.73E+03	5.73E+03	5.73E+03	4.69E+03	4.54012E-08
61	122400	1300	1.41E+05	-1.90E+04	1.90E+04	4.49E+04	4.95642E-10
68	40850	330	3.80E+04	2.81E+03	2.81E+03	1.36E+04	5.42405E-09
1718	8750	56	8.84E+03	-8.99E+01	8.99E+01	4.73E+03	4.47825E-08
BR048	391	1.4	3.02E+03	-2.63E+03	2.63E+03	2.96E+03	1.14025E-07
C-15	1348	0.099	2.88E+03	-1.53E+03	1.53E+03	2.92E+03	1.17332E-07
C-6	44710	7.58	3.68E+03	4.10E+04	4.10E+04	3.16E+03	1.00075E-07
C-8	2826	2.2	3.11E+03	-2.80E+02	2.80E+02	2.99E+03	1.1206E-07
111	5036	6.1	3.52E+03	1.51E+03	1.51E+03	3.11E+03	1.03173E-07
EPA-E3	219200	3800	4.08E+05	-1.89E+05	1.89E+05	1.26E+05	6.32999E-11
EPA-F2	77700	1188	1.29E+05	-5.18E+04	5.18E+04	4.13E+04	5.86303E-10
EPA-H1	507600	4000	4.29E+05	7.84E+04	7.84E+04	1.32E+05	5.7261E-11
GRID MARSH	3690	6.1	3.52E+03	1.68E+02	1.68E+02	3.11E+03	1.03173E-07
117	148	11	4.04E+03	-3.90E+03	3.90E+03	3.27E+03	9.34293E-08
110	630	0.25	2.90E+03	-2.27E+03	2.27E+03	2.92E+03	1.16941E-07
100	71	1.1	2.99E+03	-2.92E+03	2.92E+03	2.95E+03	1.14775E-07
101	161	0.085	2.88E+03	-2.72E+03	2.72E+03	2.92E+03	1.17368E-07
102	147	0.13	2.89E+03	-2.74E+03	2.74E+03	2.92E+03	1.17251E-07
D1-1A	1206	2.29	3.12E+03	-1.91E+03	1.91E+03	2.99E+03	1.11842E-07
D1-1B	1641	5.12	3.42E+03	-1.78E+03	1.78E+03	3.08E+03	1.05304E-07
D1-2A	565	1.37	3.02E+03	-2.45E+03	2.45E+03	2.96E+03	1.14099E-07
D1-2B	600	2.29	3.12E+03	-2.52E+03	2.52E+03	2.99E+03	1.11842E-07
D2-1A	3831	3.03	3.19E+03	6.36E+02	6.36E+02	3.01E+03	1.10075E-07
D2-1B	3162	3.22	3.21E+03	-5.28E+01	5.28E+01	3.02E+03	1.09628E-07
EC-1A	999	4.49	3.35E+03	-2.35E+03	2.35E+03	3.06E+03	1.06709E-07
EC-1B	1002	4.58	3.36E+03	-2.36E+03	2.36E+03	3.06E+03	1.06506E-07
EC-2A	2030	12.6	4.21E+03	-2.18E+03	2.18E+03	3.32E+03	9.05453E-08
EC-2B	230	5.67	3.48E+03	-3.25E+03	3.25E+03	3.10E+03	1.041E-07
EC-3A	3810	24.4	5.47E+03	-1.66E+03	1.66E+03	3.70E+03	7.28677E-08
EC-3B	20737	22.1	5.23E+03	1.55E+04	1.55E+04	3.63E+03	7.58815E-08
EC-4A	17065	28.8	5.94E+03	1.11E+04	1.11E+04	3.85E+03	6.75814E-08
EC-4B	3446	7.66	3.69E+03	-2.42E+02	2.42E+02	3.16E+03	9.99116E-08
LC-1A	728	0.721	2.95E+03	-2.22E+03	2.22E+03	2.94E+03	1.15733E-07
LC-1B	2958	0.964	2.97E+03	-1.64E+01	1.64E+01	2.95E+03	1.15117E-07
MC-1A	2089	9.35	3.87E+03	-1.78E+03	1.78E+03	3.22E+03	9.65502E-08
MC-1B	1409	2.86	3.18E+03	-1.77E+03	1.77E+03	3.01E+03	1.10477E-07
MC-2A	1515	4.98	3.40E+03	-1.89E+03	1.89E+03	3.08E+03	1.05614E-07
MC-2B	2089	14.2	4.39E+03	-2.30E+03	2.30E+03	3.37E+03	8.77928E-08
MC-3A	1358	5.68	3.48E+03	-2.12E+03	2.12E+03	3.10E+03	1.04078E-07
MC-3B	1872	18	4.79E+03	-2.92E+03	2.92E+03	3.50E+03	8.17378E-08
PC-1A	13310	31.1	6.19E+03	7.12E+03	7.12E+03	3.92E+03	6.50441E-08
PC-1B	4611	24.5	5.48E+03	-8.72E+02	8.72E+02	3.71E+03	7.27408E-08
PC-2A	649	1.24	3.00E+03	-2.35E+03	2.35E+03	2.96E+03	1.14424E-07
PC-2B	207	1.03	2.98E+03	-2.77E+03	2.77E+03	2.95E+03	1.14951E-07
PC-3A	316	1.89	3.07E+03	-2.76E+03	2.76E+03	2.98E+03	1.12815E-07
PC-3B	206	0.604	2.94E+03	-2.73E+03	2.73E+03	2.94E+03	1.16031E-07

OVERALL FIT

Multiple R	0.43602176	AIC	74.39593942
R Square	0.19011497	AICc	74.67500919
Adjusted R Square	0.17211753	BSC	76.22458081
Standard Error	2.24597172		
Observations	46		

ANOVA — Alpha 5.00E-02

	df	*SS*	*MS*	*F*	*p-value*	*sig*
Regression	1	52.10197698	52.10198	10.32870	0.00245	yes
Residual	44	221.9531151	5.04439			
Total	45	274.0550921				

	coeff	*std err*	*t stat*	*p-value*	*lower*	*upper*	*vif*
Intercept	2844.4874	1139.994327	2.50E+00	1.64E-02	5.47E+02	5.14E+03	
Ar1268 (mg/kg)	107.9829	33.59944852	3.21E+00	2.45E-03	4.03E+01	1.76E+02	1

Iteration #4

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred Y2	Residual	ABS(Res)	Pred Y2	Weight
36	14468	55	8.78E+03	5.68E+03	5.68E+03	4.73E+03	4.47E-08
61	122400	1300	1.43E+05	-2.08E+04	2.08E+04	4.50E+04	4.94E-10
68	40850	330	3.85E+04	2.37E+03	2.37E+03	1.36E+04	5.38E-09
1718	8750	56	8.89E+03	-1.42E+02	1.42E+02	4.76E+03	4.41E-08
BR048	391	1.4	3.00E+03	-2.60E+03	2.60E+03	3.00E+03	1.11E-07
C-15	1348	0.099	2.86E+03	-1.51E+03	1.51E+03	2.96E+03	1.14E-07
C-6	44710	7.58	3.66E+03	4.10E+04	4.10E+04	3.20E+03	9.78E-08
C-8	2826	2.2	3.08E+03	-2.56E+02	2.56E+02	3.02E+03	1.09E-07
111	5036	6.1	3.50E+03	1.53E+03	1.53E+03	3.15E+03	1.01E-07
EPA-E3	219200	3800	4.13E+05	-1.94E+05	1.94E+05	1.26E+05	6.31E-11
EPA-F2	77700	1188	1.31E+05	-5.34E+04	5.34E+04	4.14E+04	5.84E-10
EPA-H1	507600	4000	4.35E+05	7.28E+04	7.28E+04	1.32E+05	5.71E-11
GRID MARSH	3690	6.1	3.50E+03	1.87E+02	1.87E+02	3.15E+03	1.01E-07
117	148	11	4.03E+03	-3.88E+03	3.88E+03	3.31E+03	9.14E-08
110	630	0.25	2.87E+03	-2.24E+03	2.24E+03	2.96E+03	1.14E-07
100	71	1.1	2.96E+03	-2.89E+03	2.89E+03	2.99E+03	1.12E-07
101	161	0.085	2.85E+03	-2.69E+03	2.69E+03	2.95E+03	1.15E-07
102	147	0.13	2.86E+03	-2.71E+03	2.71E+03	2.95E+03	1.14E-07
D1-1A	1206	2.29	3.09E+03	-1.89E+03	1.89E+03	3.03E+03	1.09E-07
D1-1B	1641	5.12	3.40E+03	-1.76E+03	1.76E+03	3.12E+03	1.03E-07
D1-2A	565	1.37	2.99E+03	-2.43E+03	2.43E+03	3.00E+03	1.11E-07
D1-2B	600	2.29	3.09E+03	-2.49E+03	2.49E+03	3.03E+03	1.09E-07
D2-1A	3831	3.03	3.17E+03	6.59E+02	6.59E+02	3.05E+03	1.07E-07
D2-1B	3162	3.22	3.19E+03	-3.02E+01	3.02E+01	3.06E+03	1.07E-07
EC-1A	999	4.49	3.33E+03	-2.33E+03	2.33E+03	3.10E+03	1.04E-07
EC-1B	1002	4.58	3.34E+03	-2.34E+03	2.34E+03	3.10E+03	1.04E-07
EC-2A	2030	12.6	4.21E+03	-2.18E+03	2.18E+03	3.36E+03	8.86E-08
EC-2B	230	5.67	3.46E+03	-3.23E+03	3.23E+03	3.14E+03	1.02E-07
EC-3A	3810	24.4	5.48E+03	-1.67E+03	1.67E+03	3.74E+03	7.14E-08
EC-3B	20737	22.1	5.23E+03	1.55E+04	1.55E+04	3.67E+03	7.44E-08
EC-4A	17065	28.8	5.95E+03	1.11E+04	1.11E+04	3.88E+03	6.63E-08
EC-4B	3446	7.66	3.67E+03	-2.26E+02	2.26E+02	3.20E+03	9.77E-08
LC-1A	728	0.721	2.92E+03	-2.19E+03	2.19E+03	2.98E+03	1.13E-07
LC-1B	2958	0.964	2.95E+03	9.42E+00	9.42E+00	2.98E+03	1.12E-07
MC-1A	2089	9.35	3.85E+03	-1.77E+03	1.77E+03	3.25E+03	9.44E-08
MC-1B	1409	2.86	3.15E+03	-1.74E+03	1.74E+03	3.04E+03	1.08E-07
MC-2A	1515	4.98	3.38E+03	-1.87E+03	1.87E+03	3.11E+03	1.03E-07
MC-2B	2089	14.2	4.38E+03	-2.29E+03	2.29E+03	3.41E+03	8.59E-08
MC-3A	1358	5.68	3.46E+03	-2.10E+03	2.10E+03	3.14E+03	1.02E-07
MC-3B	1872	18	4.79E+03	-2.92E+03	2.92E+03	3.53E+03	8.00E-08
PC-1A	13310	31.1	6.20E+03	7.11E+03	7.11E+03	3.96E+03	6.38E-08
PC-1B	4611	24.5	5.49E+03	-8.79E+02	8.79E+02	3.74E+03	7.13E-08
PC-2A	649	1.24	2.98E+03	-2.33E+03	2.33E+03	2.99E+03	1.12E-07
PC-2B	207	1.03	2.96E+03	-2.75E+03	2.75E+03	2.99E+03	1.12E-07
PC-3A	316	1.89	3.05E+03	-2.73E+03	2.73E+03	3.01E+03	1.10E-07
PC-3B	206	0.604	2.91E+03	-2.70E+03	2.70E+03	2.97E+03	1.13E-07

OVERALL FIT

Multiple R	0.437960509	AIC	73.37933898
R Square	0.191809407	AICc	73.65840875
Adjusted R Square	0.173849616	BSC	75.20798038
Standard Error	2.221290341		
Observations	46		

ANOVA — Alpha 0.05

	df	*SS*	*MS*	*F*	*p-value*	*sig*
Regression	1	51.52517133	51.52517	10.4426035	0.002334	yes
Residual	44	217.1017542	4.934131			
Total	45	268.6269255				

	coeff	*std err*	*t stat*	*p-value*	*lower*	*upper*	*vif*
Intercept	**2849.971207**	**1140.304145**	2.499308	0.016248047	551.8392	5148.103	
Ar1268 (mg/kg)	**107.6954221**	**33.32674117**	3.231502	0.002334285	40.52979	174.8611	1

Case 2b: Furan Congener Concentration and Aroclor 1268 (Cumulative Data Set)

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight	Weight * X	Weight*X^2
36	14468	55	8773.22	5694.780	5694.78	4723.682393	4.48166E-08	2.46491E-06	0.00013557
61	122400	1300	142854.02	-20454.021	20454.02	44994.11531	4.93956E-10	6.42143E-07	0.000834786
68	40850	330	38389.46	2460.539	2460.54	13618.75794	5.39169E-09	1.77926E-06	0.000587155
1718	8750	56	8880.91	-130.915	130.91	4756.028122	4.4209E-08	2.47571E-06	0.00013864
BR048	391	1.4	3000.74	-2609.745	2609.74	2989.951306	1.11859E-07	1.56603E-07	2.19244E-07
C-15	1348	0.099	2860.63	-1512.633	1512.63	2947.869512	1.15076E-07	1.13925E-08	1.12786E-09
C-6	44710	7.58	3666.30	41043.697	41043.70	3189.847912	9.82788E-08	7.44954E-07	5.64675E-06
C-8	2826	2.2	3086.90	-260.901	260.90	3015.827889	1.09948E-07	2.41885E-07	5.32148E-07
111	5036	6.1	3506.91	1529.168	1529.17	3141.976233	1.01296E-07	6.17908E-07	3.76924E-06
EPA-E3	219200	3800	412092.58	-192892.575	192892.58	125858.4384	6.31299E-11	2.39894E-07	0.000911596
EPA-F2	77700	1188	130792.13	-53092.133	53092.13	41371.39363	5.84251E-10	6.94091E-07	0.00082458
EPA-H1	507600	4000	433631.66	73968.340	73968.34	132327.5843	5.71083E-11	2.28433E-07	0.000913733
GRID MARSH	3690	6.1	3506.91	183.087	183.09	3141.976233	1.01296E-07	6.17908E-07	3.76924E-06
117	148	11	4034.62	-3887.013	3887.01	3300.470306	9.18012E-08	1.00981E-06	1.11079E-05
110	630	0.25	2876.90	-2246.895	2246.90	2952.753717	1.14695E-07	2.86738E-08	7.16846E-09
100	71	1.1	2968.44	-2897.936	2897.94	2980.247587	1.12589E-07	1.23848E-07	1.36232E-07
101	161	0.085	2859.13	-2698.026	2698.03	2947.416672	1.15111E-07	9.78444E-09	8.31677E-10
102	147	0.13	2863.97	-2716.620	2716.62	2948.872229	1.14997E-07	1.49497E-08	1.94346E-09
D1-1A	1206	2.29	3096.59	-1890.594	1890.59	3018.739005	1.09736E-07	2.51295E-07	5.75466E-07
D1-1B	1641	5.12	3401.37	-1760.372	1760.37	3110.277418	1.03372E-07	5.29263E-07	2.70983E-06
D1-2A	565	1.37	2997.51	-2433.014	2433.01	2988.980934	1.11932E-07	1.53347E-07	2.10085E-07
D1-2B	600	2.29	3096.59	-2496.194	2496.19	3018.739005	1.09736E-07	2.51295E-07	5.75466E-07
D2-1A	3831	3.03	3176.29	654.712	654.71	3042.674844	1.08016E-07	3.27289E-07	9.91686E-07
D2-1B	3162	3.22	3196.75	-34.750	34.75	3048.820533	1.07581E-07	3.46411E-07	1.11544E-06
EC-1A	999	4.49	3333.52	-2334.324	2334.32	3089.899609	1.0474E-07	4.70281E-07	2.11156E-06
EC-1B	1002	4.58	3343.22	-2341.516	2341.52	3092.810725	1.04543E-07	4.78805E-07	2.19293E-06
EC-2A	2030	12.6	4206.93	-2176.934	2176.93	3352.223473	8.89885E-08	1.12126E-06	1.41278E-05
EC-2B	230	5.67	3460.60	-3230.704	3230.70	3128.067569	1.02199E-07	5.7947E-07	3.28559E-06
EC-3A	3810	24.4	5477.74	-1667.740	1667.74	3733.903078	7.17256E-08	1.7501E-06	4.27025E-05
EC-3B	20737	22.1	5230.04	15506.960	15506.96	3659.507901	7.46715E-08	1.65024E-06	3.64703E-05
EC-4A	17065	28.8	5951.60	11113.401	11113.40	3876.224287	6.65552E-08	1.91679E-06	5.52036E-05
EC-4B	3446	7.66	3674.92	-228.918	228.92	3192.435571	9.81196E-08	7.51596E-07	5.75723E-06
LC-1A	728	0.721	2927.62	-2199.420	2199.42	2967.988555	1.13521E-07	8.18485E-08	5.90128E-08
LC-1B	2958	0.964	2953.79	4.210	4.21	2975.848568	1.12922E-07	1.08857E-07	1.04938E-07
MC-1A	2089	9.35	3856.92	-1767.923	1767.92	3247.099853	9.48437E-08	8.86789E-07	8.29148E-06
MC-1B	1409	2.86	3157.98	-1748.980	1748.98	3037.17607	1.08408E-07	3.10046E-07	8.86731E-07
MC-2A	1515	4.98	3386.29	-1871.294	1871.29	3105.749016	1.03673E-07	5.16293E-07	2.57114E-06
MC-2B	2089	14.2	4379.25	-2290.246	2290.25	3403.97664	8.63032E-08	1.22551E-06	1.74022E-05
MC-3A	1358	5.68	3461.68	-2103.681	2103.68	3128.391027	1.02178E-07	5.80372E-07	3.29651E-06
MC-3B	1872	18	4788.49	-2916.489	2916.49	3526.890411	8.03926E-08	1.44707E-06	2.60472E-05
PC-1A	13310	31.1	6199.30	7110.701	7110.70	3950.619464	6.40722E-08	1.99265E-06	6.19713E-05
PC-1B	4611	24.5	5488.51	-877.509	877.51	3737.137651	7.16014E-08	1.75424E-06	4.29788E-05
PC-2A	649	1.24	2983.51	-2334.214	2334.21	2984.775989	1.12247E-07	1.39187E-07	1.72592E-07
PC-2B	207	1.03	2960.90	-2754.197	2754.20	2977.983386	1.1276E-07	1.16143E-07	1.19627E-07
PC-3A	316	1.89	3053.52	-2737.316	2737.32	3005.800713	1.10683E-07	2.0919E-07	3.9537E-07
PC-3B	206	0.604	2915.02	-2708.819	2708.82	2964.204105	1.13811E-07	6.87418E-08	4.152E-08
						SUM	4.0319E-06	3.21165E-05	0.004703619

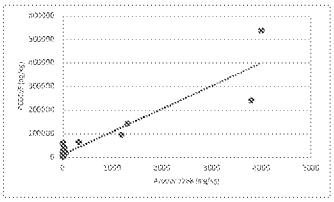
WLS Error Variance **225**

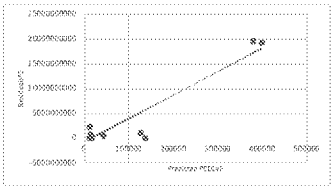
$$Var = \frac{\sum w_i}{\left((\sum w_i)(\sum w_i x_i^2) - (\sum w_i x_i)^2\right)}$$

WLS Var:OLS Var = **1.09**
Heteroscedasticity not severe

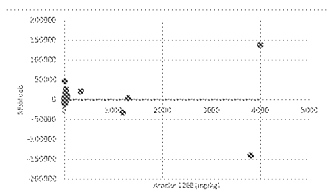
Case 3a: PCDD/F Concentration and Aroclor 1268 (Original Distribution)

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)	Pred PCDD/F (ng/kg)	Pred PCDD/F^2	Residual PCDD/F	Residual^2
36	27038	55	16341.85	267056024.49	10696.05	114405506.42
61	141906	1300	137293.72	18849566843.40	4612.27	21273071.49
68	64192	330	43058.13	1854002271.89	21133.87	446640560.85
1718	18409	56	16439.00	270240687.17	1970.20	3881692.57
BR048	2981	1.4	11134.60	123979394.05	-8153.60	66481249.15
C-15	10834	0.099	11008.21	121180713.19	-174.21	30349.55
C-6	59189	7.58	11734.99	137710015.58	47454.01	2251882882.02
111	9396	6.1	11591.21	134356124.40	-2194.84	4817331.09
EPA-E3	240328	3800	380168.98	144528451366.68	-139840.78	19555443019.91
EPA-F2	94088	1188	126412.91	15980224670.48	-32325.21	1044919420.38
EPA-H1	538204	4000	399599.00	159679359883.26	138605.20	19211402132.23
GRID MARSH	5980	6.1	11591.21	134356124.40	-5611.21	31485666.88
117	2133	11	12067.24	145618387.96	-9933.83	98680996.80
110	3049	0.25	11022.88	121503901.93	-7974.28	63589154.86
100	856	1.1	11105.46	123331206.77	-10249.76	105057547.71
101	2058	0.085	11006.85	121150770.47	-8949.26	80089202.10
102	2678	0.13	11011.22	121247028.08	-8333.21	69442319.31
D2-1A	10471	3.03	11292.96	127530903.04	-822.36	676272.87
D2-1B	8782	3.22	11311.42	127948146.32	-2529.32	6397442.65
EC-3A	9344	24.4	13369.06	178731652.37	-4025.36	16203489.13
EC-3B	31228	22.1	13145.61	172807076.59	18082.79	326987274.48
EC-4A	26257	28.8	13796.52	190343859.86	12460.68	155268640.22
EC-4B	9798	7.66	11742.76	137892484.88	-1944.46	3780936.69
LC-1A	6839	0.721	11068.64	122514758.99	-4229.94	17892380.00
LC-1B	15394	0.964	11092.25	123037921.51	4301.55	18503366.74
PC-1A	40766	31.1	14019.96	196559319.18	26746.34	715366625.60
PC-1B	18361	24.5	13378.77	178991507.78	4982.03	24820615.08
PC-2A	3534	1.24	11119.06	123633482.75	-7584.66	57527058.77
PC-2B	3473	1.03	11098.66	123180207.52	-7625.36	58146083.33
PC-3A	1691	1.89	11182.21	125041753.44	-9491.21	90083010.36
PC-3B	1128	0.604	11057.27	122263263.46	-9929.70	98598981.25
D1-2A	6945	1.37	11131.69	123914498.87	-4186.79	17529201.71
D1-2B	6285	2.29	11221.07	125912345.57	-4935.67	24360809.15





Test for Zero Conditional Mean of Errors



No discernable relationship between residuals and independent variable
$Cov(\hat{u}_i, x_i) = 0$

Tests for Homoscedasticity

BREUSCH-PAGAN SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.951750162
R Square	0.905828371
Adjusted R Square	0.902790576
Standard Error	1455898725
Observations	33

$$\hat{u}^2 = d_0 + x d_1$$

H_0 = homoscedasticity of residuals
H_a = heteroscedasticity of residuals
$p<0.05$
Status: Heteroscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	6.32048E+20	6.32048E+20	298.1861914	1.85625E-17
Residual	31	6.57089E+19	2.11964E+18		
Total	32	6.97757E+20			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-159722894.1	268240051.2	-0.595447598	0.555866788	-706802085.3	387356297.1	-706802085.3	387356297.1
Ar1268 (mg/kg)	4586335.112	265596.2999	17.26806855	1.85625E-17	4044647.888	5128022.337	4044647.888	5128022.337

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.992866026
R Square	0.985782946
Adjusted R Square	0.984825143
Standard Error	575037466.9
Observations	33

$$\hat{u}^2 = d_0 + \hat{Y} \times d_1 + \hat{Y}^2 \times d_2$$

H_0 = homoscedasticity of residuals
H_a = heteroscedasticity of residuals
$p<0.05$
Status: Heteroscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	2	6.87837E+20	3.43918E+20	1040.070938	1.95949E-28
Residual	30	9.92004E+18	3.30668E+17		
Total	32	6.97757E+20			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	388823146.1	137651625.4	2.824689828	0.008333454	107701023	669945269.3	107701023	669945269.3
Pred PCDD/F (ng/kg)	-20202.32708	5300.9799	-3.811055213	0.000640041	-31028.37232	-9376.28184	-31028.37232	-9376.28184
Pred PCDD/F^2	0.176024473	0.013551756	12.98905303	7.52072E-14	0.148348095	0.20370085	0.148348095	0.20370085

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y^	Weight	Weight * X	Weight*X^2
36	27038	55	16341.85	10696.051	10696.05	8938.760164	1.25154E-08	6.88348E-07	3.78591E-05
61	141906	1300	137293.72	4612.274	4612.27	48207.39744	4.30301E-10	5.59392E-07	0.000727209
68	64192	330	43058.13	21133.872	21133.87	17612.55555	3.2237E-09	1.06382E-06	0.000351061
1718	18409	56	16439.00	1970.201	1970.20	8970.301238	1.24276E-08	6.95943E-07	3.89728E-05
BR048	2981	1.4	11134.60	-8153.603	8153.60	7248.158591	1.90346E-08	2.66485E-08	3.73079E-08
C-15	10834	0.099	11008.21	-174.211	174.21	7207.123654	1.9252E-08	1.90595E-09	1.88689E-10
C-6	59189	7.58	11734.99	47454.008	47454.01	7443.082429	1.80507E-08	1.36824E-07	1.03713E-06
111	9396	6.1	11591.21	-2194.842	2194.84	7396.40164	1.82793E-08	1.11504E-07	6.80172E-07
EPA-E3	240328	3800	380168.98	-139840.777	139840.78	127060.0827	6.19415E-11	2.35378E-07	0.000894435
EPA-F2	94088	1188	126412.91	-32325.213	32325.21	44674.79714	5.01043E-10	5.95239E-07	0.000707144
EPA-H1	538204	4000	399599.00	138605.202	138605.20	133368.2976	5.62205E-11	2.24882E-07	0.000899528
GRID MARSH	5980	6.1	11591.21	-5611.209	5611.21	7396.40164	1.82793E-08	1.11504E-07	6.80172E-07
117	2133	11	12067.24	-9933.831	9933.83	7550.952903	1.75387E-08	1.92925E-07	2.12218E-06
110	3049	0.25	11022.88	-7974.281	7974.28	7211.886356	1.92266E-08	4.80665E-09	1.20166E-09
100	856	1.1	11105.46	-10249.758	10249.76	7238.696269	1.90844E-08	2.09929E-08	2.30922E-08
101	2058	0.085	11006.85	-8949.257	8949.26	7206.682079	1.92544E-08	1.63662E-09	1.39113E-10
102	2678	0.13	11011.22	-8333.206	8333.21	7208.101427	1.92468E-08	2.50208E-09	3.25271E-10
D2-1A	10471	3.03	11292.96	-822.358	822.36	7299.570542	1.87675E-08	5.68654E-08	1.72302E-07
D2-1B	8782	3.22	11311.42	-2529.317	2529.32	7305.563346	1.87367E-08	6.03321E-08	1.94269E-07
EC-3A	9344	24.4	13369.06	-4025.356	4025.36	7973.603296	1.57286E-08	3.83778E-07	9.36419E-06
EC-3B	31228	22.1	13145.61	18082.789	18082.79	7901.058826	1.60188E-08	3.54015E-07	7.82373E-06
EC-4A	26257	28.8	13796.52	12460.684	12460.68	8112.384022	1.51951E-08	4.37618E-07	1.26034E-05
EC-4B	9798	7.66	11742.76	-1944.463	1944.46	7445.605715	1.80385E-08	1.38175E-07	1.05842E-06
LC-1A	6839	0.721	11068.64	-4229.939	4229.94	7226.742202	1.91476E-08	1.38054E-08	9.95372E-09
LC-1B	15394	0.964	11092.25	4301.554	4301.55	7234.406683	1.91071E-08	1.84192E-08	1.77561E-08
PC-1A	40766	31.1	14019.96	26746.339	26746.34	8184.928493	1.49269E-08	4.64227E-07	1.44375E-05
PC-1B	18361	24.5	13378.77	4982.029	4982.03	7976.757403	1.57162E-08	3.85047E-07	9.43364E-06
PC-2A	3534	1.24	11119.06	-7584.659	7584.66	7243.112019	1.90612E-08	2.36359E-08	2.93085E-08
PC-2B	3473	1.03	11098.66	-7625.358	7625.36	7236.488394	1.90961E-08	1.9669E-08	2.0259E-08
PC-3A	1691	1.89	11182.21	-9491.207	9491.21	7263.613718	1.89537E-08	3.58225E-08	6.77046E-08
PC-3B	1128	0.604	11057.27	-9929.702	9929.70	7223.051896	1.91672E-08	1.1577E-08	6.9925E-09
D1-2A	6945	1.37	11131.69	-4186.789	4186.79	7247.212359	1.90396E-08	2.60843E-08	3.57354E-08
D1-2B	6285	2.29	11221.07	-4935.667	4935.67	7276.230147	1.88881E-08	4.32536E-08	9.90508E-08
						SUM	5.02052E-07	7.14658E-06	0.003716166

OLS Error Variance **277**

$$Var = \frac{\sum w_i}{\left((\sum w_i)(\sum w_i x_i^2) - (\sum w_i x_i)^2\right)}$$

Case 3a: PCDD/F Concentration and Aroclor 1268 (Original Distribution)

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)
36	27038	55
61	141906	1300
68	64192	330
1718	18409	56
BR048	2981	1.4
C-15	10834	0.099
C-6	59189	7.58
111	9396	6.1
EPA-E3	240328	3800
EPA-F2	94088	1188
EPA-H1	538204	4000
GRID MARSH	5980	6.1
117	2133	11
110	3049	0.25
100	856	1.1
101	2058	0.085
102	2678	0.13
D2-1A	10471	3.03
D2-1B	8782	3.22
EC-3A	9344	24.4
EC-3B	31228	22.1
EC-4A	26257	28.8
EC-4B	9798	7.66
LC-1A	6839	0.721
LC-1B	15394	0.964
PC-1A	40766	31.1
PC-1B	18361	24.5
PC-2A	3534	1.24
PC-2B	3473	1.03
PC-3A	1691	1.89
PC-3B	1128	0.604
D1-2A	6945	1.37
D1-2B	6285	2.29

Weighted Least Squares performed with "Real Stats" Add-In

$$Pred\ Y_i' = Abs(Res)x + \partial_1$$

$$W_i = \frac{1}{Pred\ Y_i'^2}$$

WLS solution is asymptotic at Iteration #4.

Iteration #1

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight
36	27038	55	1.63E+04	1.07E+04	1.07E+04	8.94E+03	1.25154E-08
61	141906	1300	1.37E+05	4.61E+03	4.61E+03	4.82E+04	4.30301E-10
68	64192	330	4.31E+04	2.11E+04	2.11E+04	1.76E+04	3.2237E-09
1718	18409	56	1.64E+04	1.97E+03	1.97E+03	8.97E+03	1.24276E-08
BR048	2981	1.4	1.11E+04	-8.15E+03	8.15E+03	7.25E+03	1.90346E-08
C-15	10834	0.099	1.10E+04	-1.74E+02	1.74E+02	7.21E+03	1.9252E-08
C-6	59189	7.58	1.17E+04	4.75E+04	4.75E+04	7.44E+03	1.80507E-08
111	9396	6.1	1.16E+04	-2.19E+03	2.19E+03	7.40E+03	1.82793E-08
EPA-E3	240328	3800	3.80E+05	-1.40E+05	1.40E+05	1.27E+05	6.19415E-11
EPA-F2	94088	1188	1.26E+05	-3.23E+04	3.23E+04	4.47E+04	5.01043E-10
EPA-H1	538204	4000	4.00E+05	1.39E+05	1.39E+05	1.33E+05	5.62205E-11
GRID MARSH	5980	6.1	1.16E+04	-5.61E+03	5.61E+03	7.40E+03	1.82793E-08
117	2133	11	1.21E+04	-9.93E+03	9.93E+03	7.55E+03	1.75387E-08
110	3049	0.25	1.10E+04	-7.97E+03	7.97E+03	7.21E+03	1.92268E-08
100	856	1.1	1.11E+04	-1.02E+04	1.02E+04	7.24E+03	1.90844E-08
101	2058	0.085	1.10E+04	-8.95E+03	8.95E+03	7.21E+03	1.92544E-08
102	2678	0.13	1.10E+04	-8.33E+03	8.33E+03	7.21E+03	1.92468E-08
D2-1A	10471	3.03	1.13E+04	-8.22E+02	8.22E+02	7.30E+03	1.87675E-08
D2-1B	8782	3.22	1.13E+04	-2.53E+03	2.53E+03	7.31E+03	1.87367E-08
EC-3A	9344	24.4	1.34E+04	-4.03E+03	4.03E+03	7.97E+03	1.57286E-08
EC-3B	31228	22.1	1.31E+04	1.81E+04	1.81E+04	7.90E+03	1.60188E-08
EC-4A	26257	28.8	1.38E+04	1.25E+04	1.25E+04	8.11E+03	1.51951E-08
EC-4B	9798	7.66	1.17E+04	-1.94E+03	1.94E+03	7.45E+03	1.80385E-08
LC-1A	6839	0.721	1.11E+04	-4.23E+03	4.23E+03	7.23E+03	1.91476E-08
LC-1B	15394	0.964	1.11E+04	4.30E+03	4.30E+03	7.23E+03	1.91071E-08
PC-1A	40766	31.1	1.40E+04	2.67E+04	2.67E+04	8.18E+03	1.49269E-08
PC-1B	18361	24.5	1.34E+04	4.98E+03	4.98E+03	7.98E+03	1.57162E-08
PC-2A	3534	1.24	1.11E+04	-7.58E+03	7.58E+03	7.24E+03	1.90612E-08
PC-2B	3473	1.03	1.11E+04	-7.63E+03	7.63E+03	7.24E+03	1.90961E-08
PC-3A	1691	1.89	1.12E+04	-9.49E+03	9.49E+03	7.26E+03	1.89537E-08
PC-3B	1128	0.604	1.11E+04	-9.93E+03	9.93E+03	7.22E+03	1.91672E-08
D1-2A	6945	1.37	1.11E+04	-4.19E+03	4.19E+03	7.25E+03	1.90396E-08
D1-2B	6285	2.29	1.12E+04	-4.94E+03	4.94E+03	7.28E+03	1.88881E-08

OVERALL FIT			
Multiple R	0.58417537	AIC	32.06906335
R Square	0.34126086	AICc	32.46906335
Adjusted R Square	0.32067527	BSC	33.56557091
Standard Error	1.62718585		
Observations	33		

ANOVA	df	SS	MS	F	Alpha 5.00E-02 p-value	sig
Regression	1	42.52154429	42.52154	16.05960	0.00036	yes
Residual	31	82.07974702	2.64773			
Total	32	124.6012913				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	10586.7001	2328.574909	4.55E+00	7.85E-05	5.84E+03	1.53E+04	
Ar1268 (mg/kg)	108.4637	27.06555148	4.01E+00	3.58E-04	5.33E+01	1.64E+02	1

Iteration #2

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)	Pred Y2	Residual	ABS(Res)	Pred Y2'	Weight
36	27038	55	1.66E+04	1.05E+04	1.05E+04	9.12E+03	1.20268E-08
61	141906	1300	1.52E+05	-9.68E+03	9.68E+03	4.84E+04	4.26171E-10
68	64192	330	4.64E+04	1.78E+04	1.78E+04	1.78E+04	3.15471E-09
1718	18409	56	1.67E+04	1.75E+03	1.75E+03	9.15E+03	1.19439E-08
BR048	2981	1.4	1.07E+04	-7.76E+03	7.76E+03	7.43E+03	1.81355E-08
C-15	10834	0.099	1.06E+04	2.37E+02	2.37E+02	7.38E+03	1.83379E-08
C-6	59189	7.58	1.14E+04	4.78E+04	4.78E+04	7.62E+03	1.72184E-08
111	9396	6.1	1.12E+04	-1.85E+03	1.85E+03	7.57E+03	1.74316E-08
EPA-E3	240328	3800	4.23E+05	-1.82E+05	1.82E+05	1.27E+05	6.16113E-11
EPA-F2	94088	1188	1.39E+05	-4.54E+04	4.54E+04	4.49E+04	4.95962E-10
EPA-H1	538204	4000	4.44E+05	9.38E+04	9.38E+04	1.34E+05	5.59278E-11
GRID MARSH	5980	6.1	1.12E+04	-5.27E+03	5.27E+03	7.57E+03	1.74316E-08
117	2133	11	1.18E+04	-9.65E+03	9.65E+03	7.73E+03	1.67405E-08
110	3049	0.25	1.06E+04	-7.57E+03	7.57E+03	7.39E+03	1.83143E-08
100	856	1.1	1.07E+04	-9.85E+03	9.85E+03	7.42E+03	1.81819E-08
101	2058	0.085	1.06E+04	-8.54E+03	8.54E+03	7.38E+03	1.83401E-08
102	2678	0.13	1.06E+04	-7.92E+03	7.92E+03	7.39E+03	1.83331E-08
D2-1A	10471	3.03	1.09E+04	-4.45E+02	4.45E+02	7.48E+03	1.78867E-08
D2-1B	8782	3.22	1.09E+04	-2.15E+03	2.15E+03	7.48E+03	1.7858E-08
EC-3A	9344	24.4	1.32E+04	3.89E+03	3.89E+03	8.15E+03	1.50474E-08
EC-3B	31228	22.1	1.30E+04	1.82E+04	1.82E+04	8.08E+03	1.53192E-08
EC-4A	26257	28.8	1.37E+04	1.25E+04	1.25E+04	8.29E+03	1.45472E-08
EC-4B	9798	7.66	1.14E+04	-1.62E+03	1.62E+03	7.62E+03	1.7207E-08
LC-1A	6839	0.721	1.07E+04	-3.83E+03	3.83E+03	7.40E+03	1.82407E-08
LC-1B	15394	0.964	1.07E+04	4.70E+03	4.70E+03	7.41E+03	1.8203E-08
PC-1A	40766	31.1	1.40E+04	2.68E+04	2.68E+04	8.36E+03	1.42956E-08
PC-1B	18361	24.5	1.32E+04	5.12E+03	5.12E+03	8.16E+03	1.50358E-08
PC-2A	3534	1.24	1.07E+04	-7.19E+03	7.19E+03	7.42E+03	1.81602E-08
PC-2B	3473	1.03	1.07E+04	-7.23E+03	7.23E+03	7.41E+03	1.81928E-08
PC-3A	1691	1.89	1.08E+04	-9.10E+03	9.10E+03	7.44E+03	1.80602E-08
PC-3B	1128	0.604	1.07E+04	-9.52E+03	9.52E+03	7.40E+03	1.8259E-08
D1-2A	6945	1.37	1.07E+04	-3.79E+03	3.79E+03	7.42E+03	1.81402E-08
D1-2B	6285	2.29	1.08E+04	-4.55E+03	4.55E+03	7.45E+03	1.7999E-08

OVERALL FIT			
Multiple R	0.589311837	AIC	30.60638984
R Square	0.347288442	AICc	31.00638984
Adjusted R Square	0.326891205	BSC	32.1028974
Standard Error	1.591521262		
Observations	33		

ANOVA	df	SS	MS	F	Alpha 0.05 p-value	sig
Regression	1	41.77876618	41.77877	16.49417963	0.000308	yes
Residual	31	78.52113778	2.53294			
Total	32	120.299904				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	10605.64135	2331.243847	4.549349	7.78096E-05	5851.038	15360.24	
Ar1268 (mg/kg)	108.0353826	26.60118484	4.061303	0.000307981	53.78195	162.2888	1

Iteration #3

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight
36	27038	55	1.63E+04	1.05E+04	1.05E+04	9.11E+03	1.20268E-08
61	141906	1300	1.51E+05	-9.15E+03	9.15E+03	4.84E+04	4.26893E-10
68	64192	330	4.63E+04	1.79E+04	1.79E+04	1.78E+04	3.16078E-09
1718	18409	56	1.67E+04	1.75E+03	1.75E+03	9.14E+03	1.19794E-08
BR048	2981	1.4	1.08E+04	-7.78E+03	7.78E+03	7.41E+03	1.81985E-08
C-15	10834	0.099	1.06E+04	2.18E+02	2.18E+02	7.37E+03	1.84018E-08
C-6	59189	7.58	1.14E+04	4.78E+04	4.78E+04	7.61E+03	1.7277E-08
111	9396	6.1	1.13E+04	-1.87E+03	1.87E+03	7.56E+03	1.74912E-08
EPA-E3	240328	3800	4.21E+05	-1.81E+05	1.81E+05	1.27E+05	6.16713E-11
EPA-F2	94088	1188	1.39E+05	-4.49E+04	4.49E+04	4.49E+04	4.96585E-10
EPA-H1	538204	4000	4.43E+05	9.55E+04	9.55E+04	1.34E+05	5.59819E-11
GRID MARSH	5980	6.1	1.13E+04	-5.28E+03	5.28E+03	7.56E+03	1.74912E-08
117	2133	11	1.18E+04	-9.66E+03	9.66E+03	7.72E+03	1.67969E-08
110	3049	0.25	1.06E+04	-7.58E+03	7.58E+03	7.38E+03	1.83781E-08
100	856	1.1	1.07E+04	-9.87E+03	9.87E+03	7.40E+03	1.82451E-08
101	2058	0.085	1.06E+04	-8.56E+03	8.56E+03	7.37E+03	1.84041E-08
102	2678	0.13	1.06E+04	-7.94E+03	7.94E+03	7.37E+03	1.8397E-08
D2-1A	10471	3.03	1.09E+04	-4.62E+02	4.62E+02	7.46E+03	1.79484E-08
D2-1B	8782	3.22	1.10E+04	-2.17E+03	2.17E+03	7.47E+03	1.79196E-08
EC-3A	9344	24.4	1.32E+04	-3.90E+03	3.90E+03	8.14E+03	1.50961E-08
EC-3B	31228	22.1	1.30E+04	1.82E+04	1.82E+04	8.07E+03	1.53691E-08
EC-4A	26257	28.8	1.37E+04	1.25E+04	1.25E+04	8.28E+03	1.45857E-08
EC-4B	9798	7.66	1.14E+04	-1.63E+03	1.63E+03	7.61E+03	1.72656E-08
LC-1A	6839	0.721	1.07E+04	-3.84E+03	3.84E+03	7.39E+03	1.83042E-08
LC-1B	15394	0.964	1.07E+04	4.68E+03	4.68E+03	7.40E+03	1.82663E-08
PC-1A	40766	31.1	1.40E+04	2.68E+04	2.68E+04	8.35E+03	1.4341E-08
PC-1B	18361	24.5	1.33E+04	5.11E+03	5.11E+03	8.14E+03	1.50844E-08
PC-2A	3534	1.24	1.07E+04	-7.21E+03	7.21E+03	7.41E+03	1.82233E-08
PC-2B	3473	1.03	1.07E+04	-7.24E+03	7.24E+03	7.40E+03	1.8256E-08
PC-3A	1691	1.89	1.08E+04	-9.12E+03	9.12E+03	7.43E+03	1.81228E-08
PC-3B	1128	0.604	1.07E+04	-9.54E+03	9.54E+03	7.39E+03	1.83225E-08
D1-2A	6945	1.37	1.08E+04	-3.81E+03	3.81E+03	7.41E+03	1.82031E-08
D1-2B	6285	2.29	1.09E+04	-4.57E+03	4.57E+03	7.44E+03	1.80613E-08

OVERALL FIT			
Multiple R	0.58901378	AIC	30.71295874
R Square	0.34693723	AICc	31.11295874
Adjusted R Square	0.32652902	BSC	32.20946631
Standard Error	1.59409314		
Observations	33		

ANOVA	df	SS	MS	F	Alpha 5.00E-02 p-value	sig
Regression	1	41.84899789	41.84900	16.46864	0.00031	yes
Residual	31	78.77512074	2.54113			
Total	32	120.6241186				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	10604.5514	2331.087951	4.55E+00	7.78E-05	5.85E+03	1.54E+04	
Ar1268 (mg/kg)	108.0599	26.62781594	4.06E+00	3.11E-04	5.38E+01	1.62E+02	1

Iteration #4

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)	Pred Y2	Residual	ABS(Res)	Pred Y2'	Weight
36	27038	55	1.65E+04	1.05E+04	1.05E+04	9.11E+03	1.21E-08
61	141906	1300	1.51E+05	-9.18E+03	9.18E+03	4.84E+04	4.27E-10
68	64192	330	4.63E+04	1.79E+04	1.79E+04	1.78E+04	3.16E-09
1718	18409	56	1.67E+04	1.75E+03	1.75E+03	9.14E+03	1.20E-08
BR048	2981	1.4	1.08E+04	-7.77E+03	7.77E+03	7.41E+03	1.82E-08
C-15	10834	0.099	1.06E+04	2.19E+02	2.19E+02	7.37E+03	1.84E-08
C-6	59189	7.58	1.14E+04	4.78E+04	4.78E+04	7.61E+03	1.73E-08
111	9396	6.1	1.13E+04	-1.87E+03	1.87E+03	7.56E+03	1.75E-08
EPA-E3	240328	3800	4.21E+05	-1.81E+05	1.81E+05	1.27E+05	6.17E-11
EPA-F2	94088	1188	1.39E+05	-4.49E+04	4.49E+04	4.49E+04	4.97E-10
EPA-H1	538204	4000	4.43E+05	9.54E+04	9.54E+04	1.34E+05	5.60E-11
GRID MARSH	5980	6.1	1.13E+04	-5.28E+03	5.28E+03	7.56E+03	1.75E-08
117	2133	11	1.18E+04	-9.66E+03	9.66E+03	7.72E+03	1.68E-08
110	3049	0.25	1.06E+04	-7.58E+03	7.58E+03	7.38E+03	1.84E-08
100	856	1.1	1.07E+04	-9.87E+03	9.87E+03	7.40E+03	1.82E-08
101	2058	0.085	1.06E+04	-8.56E+03	8.56E+03	7.37E+03	1.84E-08
102	2678	0.13	1.06E+04	-7.94E+03	7.94E+03	7.37E+03	1.84E-08
D2-1A	10471	3.03	1.09E+04	-4.61E+02	4.61E+02	7.46E+03	1.79E-08
D2-1B	8782	3.22	1.10E+04	-2.17E+03	2.17E+03	7.47E+03	1.79E-08
EC-3A	9344	24.4	1.32E+04	-3.90E+03	3.90E+03	8.14E+03	1.51E-08
EC-3B	31228	22.1	1.30E+04	1.82E+04	1.82E+04	8.07E+03	1.54E-08
EC-4A	26257	28.8	1.37E+04	1.25E+04	1.25E+04	8.28E+03	1.46E-08
EC-4B	9798	7.66	1.14E+04	-1.63E+03	1.63E+03	7.61E+03	1.73E-08
LC-1A	6839	0.721	1.07E+04	-3.84E+03	3.84E+03	7.39E+03	1.83E-08
LC-1B	15394	0.964	1.07E+04	4.69E+03	4.69E+03	7.40E+03	1.83E-08
PC-1A	40766	31.1	1.40E+04	2.68E+04	2.68E+04	8.35E+03	1.43E-08
PC-1B	18361	24.5	1.33E+04	5.11E+03	5.11E+03	8.14E+03	1.51E-08
PC-2A	3534	1.24	1.07E+04	-7.20E+03	7.20E+03	7.41E+03	1.82E-08
PC-2B	3473	1.03	1.07E+04	-7.24E+03	7.24E+03	7.40E+03	1.83E-08
PC-3A	1691	1.89	1.08E+04	-9.12E+03	9.12E+03	7.43E+03	1.81E-08
PC-3B	1128	0.604	1.07E+04	-9.54E+03	9.54E+03	7.39E+03	1.83E-08
D1-2A	6945	1.37	1.08E+04	-3.81E+03	3.81E+03	7.41E+03	1.82E-08
D1-2B	6285	2.29	1.09E+04	-4.57E+03	4.57E+03	7.44E+03	1.81E-08

OVERALL FIT			
Multiple R	0.589030744	AIC	30.70688535
R Square	0.346957217	AICc	31.10688535
Adjusted R Square	0.32654963	BSC	32.20338291
Standard Error	1.593946453		
Observations	33		

ANOVA	df	SS	MS	F	Alpha 0.05 p-value	sig
Regression	1	4.18E+01	41.84499	16.47009048	0.000311	yes
Residual	31	78.76062411	2.540665			
Total	32	120.6056114				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	**10604.6135**	**2331.096821**	4.549195	7.78436E-05	5850.31	15358.92	
Ar1268 (mg/kg)	**108.0584622**	**26.62629812**	4.058336	0.00031054	53.75377	162.3632	1

Case 3a: PCDD/F Concentration and Aroclor 1268 (Original Distribution)

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight	Weight * X	Weight*X^2
36	27038	55	16547.83	10490.071	10490.07	9105.730375	1.20606E-08	6.63335E-07	3.64834E-05
61	141906	1300	151080.61	-9174.616	9174.62	48412.39425	4.26665E-10	5.54664E-07	0.000721064
68	64192	330	46263.91	17928.093	17928.09	17787.92521	3.16045E-09	1.04295E-06	0.000344173
1718	18409	56	16655.89	1753.313	1753.31	9137.301993	1.19774E-08	6.70737E-07	3.75613E-05
BR048	2981	1.4	10755.90	-7774.895	7774.90	7413.491674	1.81951E-08	2.54731E-08	3.56624E-08
C-15	10834	0.099	10615.31	218.689	218.69	7372.416999	1.83984E-08	1.82144E-09	1.80323E-10
C-6	59189	7.58	11423.70	47765.303	47765.30	7608.60427	1.72739E-08	1.30936E-07	9.92495E-07
111	9396	6.1	11263.77	-1867.403	1867.40	7561.878276	1.7488E-08	1.06677E-07	6.50729E-07
EPA-E3	240328	3800	421226.77	-180898.570	180898.57	127341.4382	6.16681E-11	2.34339E-07	0.000890487
EPA-F2	94088	1188	138978.07	-44890.367	44890.37	44876.37308	4.96552E-10	5.89903E-07	0.000700805
EPA-H1	538204	4000	442838.46	95365.738	95365.74	133655.7617	5.59789E-11	2.23916E-07	0.000895663
GRID MARSH	5980	6.1	11263.77	-5283.770	5283.77	7561.878276	1.7488E-08	1.06677E-07	6.50729E-07
117	2133	11	11793.26	-9659.843	9659.84	7716.579202	1.67939E-08	1.84732E-07	2.03206E-06
110	3049	0.25	10631.63	-7583.028	7583.03	7377.184313	1.83746E-08	4.59366E-09	1.14841E-09
100	856	1.1	10723.48	-9867.778	9867.78	7404.020188	1.82417E-08	2.00658E-08	2.20724E-08
101	2058	0.085	10613.80	-8556.204	8556.20	7371.974997	1.84006E-08	1.56405E-09	1.32944E-10
102	2678	0.13	10618.66	-7940.644	7940.64	7373.395719	1.83935E-08	2.39116E-09	3.10851E-10
D2-1A	10471	3.03	10932.03	-461.431	461.43	7464.95341	1.79451E-08	5.43736E-08	1.64752E-07
D2-1B	8782	3.22	10952.56	-2170.462	2170.46	7470.952018	1.79163E-08	5.76905E-08	1.85763E-07
EC-3A	9344	24.4	13241.24	-3897.540	3897.54	8139.638878	1.50935E-08	3.68281E-07	8.98606E-06
EC-3B	31228	22.1	12992.71	18235.694	18235.69	8067.024157	1.53664E-08	3.39598E-07	7.50512E-06
EC-4A	26257	28.8	13716.70	12540.503	12540.50	8278.553995	1.45912E-08	4.20227E-07	1.21025E-05
EC-4B	9798	7.66	11432.34	-1634.041	1634.04	7611.13	1.72624E-08	1.3223E-07	1.01288E-06
LC-1A	6839	0.721	10682.52	-3843.824	3843.82	7392.054545	1.83008E-08	1.31949E-08	9.5135E-09
LC-1B	15394	0.964	10708.78	4685.018	4685.02	7399.726448	1.82629E-08	1.76054E-08	1.69716E-08
PC-1A	40766	31.1	13965.23	26801.068	26801.07	8351.168715	1.43386E-08	4.45929E-07	1.38684E-05
PC-1B	18361	24.5	13252.05	5108.754	5108.75	8142.796039	1.50818E-08	3.69504E-07	9.05284E-06
PC-2A	3534	1.24	10738.61	-7204.206	7204.21	7408.440215	1.82199E-08	2.25927E-08	2.80149E-08
PC-2B	3473	1.03	10715.91	-7242.614	7242.61	7401.810175	1.82526E-08	1.88002E-08	1.93642E-08
PC-3A	1691	1.89	10808.84	-9117.844	9117.84	7428.961766	1.81194E-08	3.42457E-08	6.47243E-08
PC-3B	1128	0.604	10669.88	-9542.311	9542.31	7388.360666	1.83191E-08	1.10647E-08	6.6831E-09
D1-2A	6945	1.37	10752.65	-3807.754	3807.75	7412.544525	1.81997E-08	2.49337E-08	3.41591E-08
D1-2B	6285	2.29	10852.07	-4566.667	4566.67	7441.590413	1.8058E-08	4.13527E-08	9.46977E-08
						SUM	4.80615E-07	6.9364E-06	0.003683775

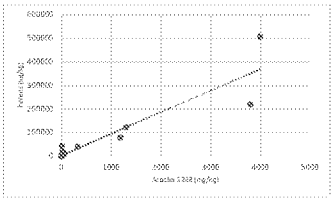
WLS Error Variance **279**

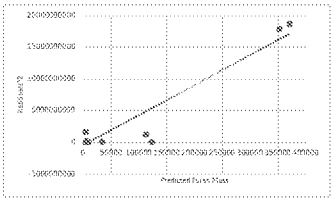
$$Var = \frac{\sum w_i}{\left((\sum w_i)(\sum w_i x_i^2) - (\sum w_i x_i)^2\right)}$$

WLS Var:OLS Var = **1.01**
Heteroscedasticity not severe

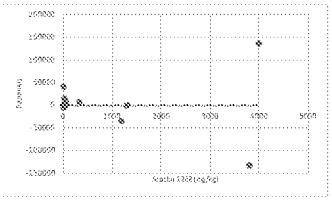
Case 3b: Furan Congener Concentration and Aroclor 1268 (Original Distribution)

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred PCDD/F (ng/kg)	Pred PCDD/F^2	Residual PCDD/F	Residual^2
36	14468	55	8709.95	75863267.95	5758.05	33155113.15
61	122400	1300	123061.00	15144010851.22	-661.01	436928.62
68	40850	330	33968.22	1153839753.42	6881.78	47358926.89
1718	8750	56	8801.80	77471691.53	-51.80	2683.28
BR048	391	1.4	3786.89	14340512.01	-3395.89	11532047.48
C-15	1348	0.099	3667.39	13449766.25	-2319.39	5379580.60
C-6	44710	7.58	4354.51	18961748.11	40355.49	1628565624.75
111	5036	6.1	4218.57	17796362.82	817.51	668318.43
EPA-E3	219200	3800	352681.59	124384305090.77	-133481.59	17817335310.17
EPA-F2	77700	1188	112774.00	12717975592.91	-35074.00	1230185636.76
EPA-H1	507600	4000	371051.24	137679021679.71	136548.76	18645564235.05
GRID MARSH	3690	6.1	4218.57	17796362.82	-528.57	279390.08
117	148	11	4668.63	21796105.18	-4521.02	20439639.05
110	630	0.25	3681.26	13551685.34	-3051.26	9310196.00
100	71	1.1	3759.33	14132579.93	-3688.83	13607484.32
101	161	0.085	3666.11	13440336.29	-3505.01	12285077.02
102	147	0.13	3670.24	13470658.66	-3522.89	12410736.98
D2-1A	3831	3.03	3936.60	15496815.40	-105.60	11151.25
D2-1B	3162	3.22	3954.05	15634516.44	-792.05	627344.21
EC-3A	3810	24.4	5899.40	34802876.12	-2089.40	4365576.69
EC-3B	20737	22.1	5688.15	32354997.07	15048.85	226468027.48
EC-4A	17065	28.8	6303.53	39734471.34	10761.47	115809269.20
EC-4B	3446	7.66	4361.86	19025794.74	-915.86	838793.68
LC-1A	728	0.721	3724.52	13872063.37	-2996.32	8977944.92
LC-1B	2958	0.964	3746.84	14038817.62	-788.84	622270.15
PC-1A	13310	31.1	6514.78	42442350.94	6795.22	46175022.68
PC-1B	4611	24.5	5908.58	34911330.30	-1297.58	1683716.64
PC-2A	649	1.24	3772.19	14229425.93	-3122.89	9752449.02
PC-2B	207	1.03	3752.90	14084280.95	-3546.20	12575555.73
PC-3A	316	1.89	3831.89	14683400.01	-3515.69	12360093.64
PC-3B	206	0.604	3713.78	13792129.61	-3507.58	12303086.97
D1-2A	565	1.37	3784.13	14319650.47	-3219.63	10366026.37
D1-2B	600	2.29	3868.63	14966311.84	-3268.23	10681335.96





Test for Zero Conditional Mean of Errors



No discernable relationship between residuals and independent variable
Cov($\hat{u}_i$, x_i) = 0

Tests for Homoscedasticity

BREUSCH-PAGAN SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.955872222
R Square	0.913691705
Adjusted R Square	0.910907566
Standard Error	1314852258
Observations	33

$$\hat{u}^2 = d_0 + x d_1$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p<0.05
Status: Heteroscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	5.67365E+20	5.67365E+20	328.1775262	4.78561E-18
Residual	31	5.35939E+19	1.72884E+18		
Total	32	6.20959E+20			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	226639094.7	242253139.4	0.935546575	0.356737866	-720717630	2674394440.5	-720717630	2674394440.5
Ar1268 (mg/kg)	4345324.653	239865.5129	18.11567074	4.78561E-18	3856115.714	4834533.592	3856115.714	4834533.592

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.996252922
R Square	0.992519884
Adjusted R Square	0.992021209
Standard Error	393482191.6
Observations	33

$$\hat{u}^2 = d_0 + \hat{Y} \times d_1 + \hat{Y}^2 \times d_2$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p<0.05
Status: Heteroscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	2	6.16314E+20	3.08157E+20	1990.316415	1.28418E-32
Residual	30	4.64485E+18	1.54828E+17		
Total	32	6.20959E+20			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	158689740.7	79912486.61	1.985794053	0.056261391	-4513329.628	321892811	-4513329.628	321892811
Pred PCDD/F (ng/kg)	-16992.14828	3699.888979	-4.592610312	7.34139E-05	-24548.32964	-9435.966927	-24548.32964	-9435.966927
Pred PCDD/F^2	0.184466108	0.010374553	17.78063223	1.76199E-17	0.163278445	0.205653772	0.163278445	0.205653772

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y^	Weight	Weight * X	Weight^X^2
36	14468	55	8709.95	5758.048	5758.05	4770.515655	4.39409E-08	2.41675E-06	0.000132921
61	122400	1300	123061.00	-661.006	661.01	44230.13175	5.11168E-10	6.64518E-07	0.000863874
68	40850	330	33968.22	6881.782	6881.78	13486.49511	5.49796E-09	1.81433E-06	0.000598728
1718	8750	56	8801.80	-51.800	51.80	4802.210126	4.33628E-08	2.42832E-06	0.000135986
BR048	391	1.4	3786.89	-3395.887	3395.89	3071.692022	1.05985E-07	1.48379E-07	2.07731E-07
C-15	1348	0.099	3667.39	-2319.392	2319.39	3030.457516	1.08889E-07	1.078E-08	1.06722E-09
C-6	44710	7.58	4354.51	40355.491	40355.49	3267.563851	9.36595E-08	7.09939E-07	5.38134E-06
111	5036	6.1	4218.57	817.507	817.51	3220.656035	9.64076E-08	5.88086E-07	3.58733E-06
EPA-E3	219200	3800	352681.59	-133481.592	133481.59	123466.3087	6.55999E-11	2.4928E-07	0.000947262
EPA-F2	77700	1188	112774.00	-35074.002	35074.00	40680.35103	6.04269E-10	7.17872E-07	0.000852832
EPA-H1	507600	4000	371051.24	136548.761	136548.76	129805.2028	5.93493E-11	2.37397E-07	0.000949589
GRID MARSH	3690	6.1	4218.57	-528.574	528.57	3220.656035	9.64076E-08	5.88086E-07	3.58733E-06
117	148	11	4668.63	-4521.022	4521.02	3375.958941	8.77416E-08	9.65158E-07	1.06167E-05
110	630	0.25	3681.26	-3051.261	3051.26	3035.243381	1.08546E-07	2.71364E-08	6.78411E-09
100	71	1.1	3759.33	-3688.832	3688.83	3062.183681	1.06644E-07	1.17309E-07	1.2904E-07
101	161	0.085	3666.11	-3505.007	3505.01	3030.013793	1.08921E-07	9.25827E-09	7.86953E-10
102	147	0.13	3670.24	-3522.888	3522.89	3031.440044	1.08818E-07	1.41464E-08	1.83903E-09
D2-1A	3831	3.03	3936.60	-105.599	105.60	3123.35401	1.02508E-07	3.10599E-07	9.41115E-07
D2-1B	3162	3.22	3954.05	-792.051	792.05	3129.375959	1.02114E-07	3.28806E-07	1.05876E-06
EC-3A	3810	24.4	5899.40	-2089.396	2089.40	3800.66485	6.92279E-08	1.68916E-06	4.12155E-05
EC-3B	20737	22.1	5688.15	15048.855	15048.85	3727.767567	7.19619E-08	1.59036E-06	3.51469E-05
EC-4A	17065	28.8	6303.53	10761.472	10761.47	3940.120521	6.44141E-08	1.85513E-06	5.34276E-05
EC-4B	3446	7.66	4361.86	-915.857	915.86	3270.099409	9.35143E-08	7.1632E-07	5.48701E-06
LC-1A	728	0.721	3724.52	-2996.322	2996.32	3050.171477	1.07486E-07	7.74973E-08	5.58756E-08
LC-1B	2958	0.964	3746.84	-788.841	788.84	3057.873233	1.06945E-07	1.03095E-07	9.93837E-08
PC-1A	13310	31.1	6514.78	6795.221	6795.22	4013.017804	6.20952E-08	1.93116E-06	6.00591E-05
PC-1B	4611	24.5	5908.58	-1297.581	1297.58	3803.834297	6.91125E-08	1.69326E-06	4.14848E-05
PC-2A	649	1.24	3772.19	-3122.891	3122.89	3066.620907	1.06336E-07	1.31856E-07	1.63502E-07
PC-2B	207	1.03	3752.90	-3546.203	3546.20	3059.965068	1.06799E-07	1.10003E-07	1.13303E-07
PC-3A	316	1.89	3831.89	-3515.692	3515.69	3087.222313	1.04921E-07	1.98301E-07	3.7479E-07
PC-3B	206	0.604	3713.78	-3507.576	3507.58	3046.463223	1.07748E-07	6.50796E-08	3.93081E-08
D1-2A	565	1.37	3784.13	-3219.631	3219.63	3070.741188	1.06051E-07	1.45289E-07	1.99047E-07
D1-2B	600	2.29	3868.63	-3268.232	3268.23	3099.900101	1.04065E-07	2.38309E-07	5.45727E-07
						SUM	2.60136E-06	2.2891E-05	0.004745124

OLS Error Variance **220**

$$Var = \frac{\sum w_i}{\left((\sum w_i)(\sum w_i x_i^2) - (\sum w_i x_i)^2\right)}$$

Case 3a: PCDD/F Concentration and Aroclor 1268 (Original Distribution)

Location	Furans (ng/kg)	Ar1268 (mg/kg)
36	14468	55
61	122400	1300
68	40850	330
1718	8750	56
BR048	391	1.4
C-15	1348	0.099
C-6	44710	7.58
111	5036	6.1
EPA-E3	219200	3800
EPA-F2	77700	1188
EPA-H1	507600	4000
GRID MARSH	3690	6.1
117	148	11
110	630	0.25
100	71	1.1
101	161	0.085
102	147	0.13
D2-1A	3831	3.03
D2-1B	3162	3.22
EC-3A	3810	24.4
EC-3B	20737	22.1
EC-4A	17065	28.8
EC-4B	3446	7.66
LC-1A	728	0.721
LC-1B	2958	0.964
PC-1A	13310	31.1
PC-1B	4611	24.5
PC-2A	649	1.24
PC-2B	207	1.03
PC-3A	316	1.89
PC-3B	206	0.604
D1-2A	565	1.37
D1-2B	600	2.29

Weighted Least Squares performed with "Real Stats" Add-In

$$Pred\ Y_i' = Abs(Res)x + \partial_1$$

$$W_i = \frac{1}{Pred\ Y_i'^2}$$

WLS solution is asymptotic at Iteration #4.

Iteration #1

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight
36	14468	55	8.71E+03	5.76E+03	5.76E+03	4.77E+03	4.39409E-08
61	122400	1300	1.23E+05	-6.61E+02	6.61E+02	4.42E+04	5.11168E-10
68	40850	330	3.40E+04	6.88E+03	6.88E+03	1.35E+04	5.49796E-09
1718	8750	56	8.80E+03	-5.18E+01	5.18E+01	4.80E+03	4.33628E-08
BR048	391	1.4	3.79E+03	-3.40E+03	3.40E+03	3.07E+03	1.05985E-07
C-15	1348	0.099	3.67E+03	-2.32E+03	2.32E+03	3.03E+03	1.08889E-07
C-6	44710	7.58	4.35E+03	4.04E+04	4.04E+04	3.27E+03	9.36595E-08
111	5036	6.1	4.22E+03	8.18E+02	8.18E+02	3.22E+03	9.64076E-08
EPA-E3	219200	3800	3.53E+05	-1.33E+05	1.33E+05	1.23E+05	6.55999E-11
EPA-F2	77700	1188	1.13E+05	-3.51E+04	3.51E+04	4.07E+04	6.04269E-10
EPA-H1	507600	4000	3.71E+05	1.37E+05	1.37E+05	1.30E+05	5.93493E-11
GRID MARSH	3690	6.1	4.22E+03	-5.29E+02	5.29E+02	3.22E+03	9.64076E-08
117	148	11	4.67E+03	-4.52E+03	4.52E+03	3.38E+03	8.77416E-08
110	630	0.25	3.68E+03	-3.05E+03	3.05E+03	3.04E+03	1.08546E-07
100	71	1.1	3.75E+03	-3.69E+03	3.69E+03	3.08E+03	1.06844E-07
101	161	0.085	3.67E+03	-3.51E+03	3.51E+03	3.03E+03	1.08921E-07
102	147	0.13	3.67E+03	-3.52E+03	3.52E+03	3.03E+03	1.08818E-07
D2-1A	3831	3.03	3.94E+03	-1.06E+02	1.06E+02	3.12E+03	1.02508E-07
D2-1B	3162	3.22	3.95E+03	-7.92E+02	7.92E+02	3.13E+03	1.02114E-07
EC-3A	3810	24.4	5.90E+03	-2.09E+03	2.09E+03	3.80E+03	6.92279E-08
EC-3B	20737	22.1	5.69E+03	1.50E+04	1.50E+04	3.73E+03	7.19619E-08
EC-4A	17065	28.8	6.30E+03	1.08E+04	1.08E+04	3.94E+03	6.44141E-08
EC-4B	3446	7.66	4.36E+03	-9.16E+02	9.16E+02	3.27E+03	9.35143E-08
LC-1A	728	0.721	3.72E+03	-3.00E+03	3.00E+03	3.05E+03	1.07486E-07
LC-1B	2958	0.964	3.75E+03	-7.89E+02	7.89E+02	3.06E+03	1.06945E-07
PC-1A	13310	31.1	6.51E+03	6.80E+03	6.80E+03	4.01E+03	6.20952E-08
PC-1B	4611	24.5	5.91E+03	-1.30E+03	1.30E+03	3.80E+03	6.91125E-08
PC-2A	649	1.24	3.77E+03	-3.12E+03	3.12E+03	3.07E+03	1.06336E-07
PC-2B	207	1.03	3.75E+03	-3.55E+03	3.55E+03	3.06E+03	1.06799E-07
PC-3A	316	1.89	3.83E+03	-3.52E+03	3.52E+03	3.09E+03	1.04921E-07
PC-3B	206	0.604	3.71E+03	-3.51E+03	3.51E+03	3.05E+03	1.07748E-07
D1-2A	565	1.37	3.78E+03	-3.22E+03	3.22E+03	3.07E+03	1.06051E-07
D1-2B	600	2.29	3.87E+03	-3.27E+03	3.27E+03	3.10E+03	1.04065E-07

OVERALL FIT			
Multiple R	0.44961362	AIC	61.52760290
R Square	0.20215241	AICc	61.92760290
Adjusted R Square	0.17721967	BSC	63.02411046
Standard Error	2.54261621		
Observations	33		

ANOVA				Alpha	5.00E-02	
	df	*SS*	*MS*	*F*	*p-value*	*sig*
Regression	1	50.77878362	50.77878	7.85454	0.00866	yes
Residual	31	200.4118133	6.46490			
Total	32	251.1905969				

	coeff	*std err*	*t stat*	*p-value*	*lower*	*upper*	*vif*
Intercept	3849.9221	1611.016205	2.39E+00	2.31E-02	5.64E+02	7.14E+03	
Ar1268 (mg/kg)	105.7150	37.72040404	2.80E+00	8.66E-03	2.88E+01	1.83E+02	1

Iteration #2

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred Y2	Residual	ABS(Res)	Pred Y2'	Weight
36	14468	55	9.66E+03	4.80E+03	4.80E+03	5.60E+03	3.19114E-08
61	122400	1300	1.41E+05	-1.89E+04	1.89E+04	4.55E+04	4.83478E-10
68	40850	330	3.87E+04	2.11E+03	2.11E+03	1.44E+04	4.81783E-09
1718	8750	56	9.77E+03	-1.02E+03	1.02E+03	5.63E+03	3.15493E-08
BR048	391	1.4	4.00E+03	3.61E+03	3.61E+03	3.88E+03	6.63931E-08
C-15	1348	0.099	3.86E+03	-2.51E+03	2.51E+03	3.84E+03	6.78423E-08
C-6	44710	7.58	4.65E+03	4.01E+04	4.01E+04	4.08E+03	6.01049E-08
111	5036	6.1	4.49E+03	5.41E+02	5.41E+02	4.03E+03	6.15268E-08
EPA-E3	219200	3800	4.08E+05	-1.86E+05	1.86E+05	1.26E+05	6.34287E-11
EPA-F2	77700	1188	1.29E+05	-5.17E+04	5.17E+04	4.19E+04	5.69837E-10
EPA-H1	507600	4000	4.27E+05	8.09E+04	8.09E+04	1.32E+05	5.74197E-11
GRID MARSH	3690	6.1	4.49E+03	-8.05E+02	8.05E+02	4.03E+03	6.15268E-08
117	148	11	5.01E+03	-4.87E+03	4.87E+03	4.19E+03	5.70018E-08
110	630	0.25	3.88E+03	-3.25E+03	3.25E+03	3.84E+03	6.76717E-08
100	71	1.1	3.97E+03	-3.90E+03	3.90E+03	3.87E+03	6.67231E-08
101	161	0.085	3.86E+03	-3.70E+03	3.70E+03	3.84E+03	6.78581E-08
102	147	0.13	3.86E+03	-3.72E+03	3.72E+03	3.84E+03	6.78072E-08
D2-1A	3831	3.03	4.17E+03	-3.39E+02	3.39E+02	3.93E+03	6.4642E-08
D2-1B	3162	3.22	4.19E+03	-1.03E+03	1.03E+03	3.94E+03	6.44424E-08
EC-3A	3810	24.4	6.43E+03	-2.62E+03	2.62E+03	4.62E+03	4.68971E-08
EC-3B	20737	22.1	6.19E+03	1.46E+04	1.46E+04	4.54E+03	4.84302E-08
EC-4A	17065	28.8	6.89E+03	1.02E+04	1.02E+04	4.76E+03	4.41602E-08
EC-4B	3446	7.66	4.66E+03	-1.21E+03	1.21E+03	4.08E+03	6.00294E-08
LC-1A	728	0.721	3.93E+03	-3.20E+03	3.20E+03	3.86E+03	6.71436E-08
LC-1B	2958	0.964	3.95E+03	-9.94E+02	9.94E+02	3.87E+03	6.68735E-08
PC-1A	13310	31.1	7.14E+03	6.17E+03	6.17E+03	4.83E+03	4.28238E-08
PC-1B	4611	24.5	6.44E+03	-1.83E+03	1.83E+03	4.62E+03	4.68321E-08
PC-2A	649	1.24	3.98E+03	-3.33E+03	3.33E+03	3.88E+03	6.65688E-08
PC-2B	207	1.03	3.96E+03	-3.75E+03	3.75E+03	3.87E+03	6.68005E-08
PC-3A	316	1.89	4.05E+03	-3.73E+03	3.73E+03	3.90E+03	6.58593E-08
PC-3B	206	0.604	3.91E+03	-3.71E+03	3.71E+03	3.86E+03	6.72742E-08
D1-2A	565	1.37	3.99E+03	-3.43E+03	3.43E+03	3.88E+03	6.6426E-08
D1-2B	600	2.29	4.09E+03	-3.49E+03	3.49E+03	3.91E+03	6.54283E-08

OVERALL FIT			
Multiple R	0.494858594	AIC	47.4034508
R Square	0.244885028	AICc	47.8034508
Adjusted R Square	0.221287685	BSC	48.89995836
Standard Error	2.052772362		
Observations	33		

ANOVA				Alpha	0.05	
	df	*SS*	*MS*	*F*	*p-value*	*sig*
Regression	1	42.3635582	42.36356	10.05335102	0.003415	yes
Residual	31	130.6301055	4.213874			
Total	32	172.9936637				

	coeff	*std err*	*t stat*	*p-value*	*lower*	*upper*	*vif*
Intercept	3991.671223	1621.546922	2.461644	0.019595118	684.5045	7298.838	
Ar1268 (mg/kg)	100.5197161	31.70266926	3.170702	0.003414783	35.8617	165.1777	1

Iteration #3

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight
36	14468	55	9.52E+03	4.95E+03	4.95E+03	5.41E+03	3.42285E-08
61	122400	1300	1.35E+05	-1.23E+04	1.23E+04	4.51E+04	4.91729E-10
68	40850	330	3.72E+04	3.69E+03	3.69E+03	1.42E+04	4.97883E-09
1718	8750	56	9.62E+03	-8.71E+02	8.71E+02	5.44E+03	3.38283E-08
BR048	391	1.4	4.13E+03	-3.74E+03	3.74E+03	3.70E+03	7.31903E-08
C-15	1348	0.099	4.00E+03	-2.65E+03	2.65E+03	3.65E+03	7.48608E-08
C-6	44710	7.58	4.75E+03	4.00E+04	4.00E+04	3.89E+03	6.59703E-08
111	5036	6.1	4.60E+03	4.31E+02	4.31E+02	3.85E+03	6.75988E-08
EPA-E3	219200	3800	3.86E+05	-1.67E+05	1.67E+05	1.25E+05	6.42092E-11
EPA-F2	77700	1188	1.23E+05	-4.57E+04	4.57E+04	4.15E+04	5.79928E-10
EPA-H1	507600	4000	4.05E+05	1.02E+05	1.02E+05	1.31E+05	5.81187E-11
GRID MARSH	3690	6.1	4.60E+03	-9.15E+02	9.15E+02	3.85E+03	6.75988E-08
117	148	11	5.10E+03	-4.95E+03	4.95E+03	4.00E+03	6.2425E-08
110	630	0.25	4.02E+03	-3.39E+03	3.39E+03	3.66E+03	7.4664E-08
100	71	1.1	4.10E+03	-4.03E+03	4.03E+03	3.69E+03	7.35705E-08
101	161	0.085	4.00E+03	-3.84E+03	3.84E+03	3.65E+03	7.48791E-08
102	147	0.13	4.00E+03	-3.86E+03	3.86E+03	3.66E+03	7.48204E-08
D2-1A	3831	3.03	4.30E+03	-4.65E+02	4.65E+02	3.75E+03	7.1175E-08
D2-1B	3162	3.22	4.32E+03	-1.15E+03	1.15E+03	3.75E+03	7.09455E-08
EC-3A	3810	24.4	6.44E+03	-2.63E+03	2.63E+03	4.43E+03	5.0965E-08
EC-3B	20737	22.1	6.21E+03	1.45E+04	1.45E+04	4.36E+03	5.26951E-08
EC-4A	17065	28.8	6.89E+03	1.02E+04	1.02E+04	4.57E+03	4.78843E-08
EC-4B	3446	7.66	4.76E+03	-1.32E+03	1.32E+03	3.90E+03	6.58839E-08
LC-1A	728	0.721	4.06E+03	-3.34E+03	3.34E+03	3.67E+03	7.40551E-08
LC-1B	2958	0.964	4.09E+03	-1.13E+03	1.13E+03	3.68E+03	7.37438E-08
PC-1A	13310	31.1	7.12E+03	6.19E+03	6.19E+03	4.64E+03	4.63838E-08
PC-1B	4611	24.5	6.45E+03	-1.84E+03	1.84E+03	4.43E+03	5.08917E-08
PC-2A	649	1.24	4.12E+03	-3.47E+03	3.47E+03	3.69E+03	7.33927E-08
PC-2B	207	1.03	4.10E+03	-3.89E+03	3.89E+03	3.68E+03	7.36596E-08
PC-3A	316	1.89	4.18E+03	-3.87E+03	3.87E+03	3.71E+03	7.25755E-08
PC-3B	206	0.604	4.05E+03	-3.85E+03	3.85E+03	3.67E+03	7.42057E-08
D1-2A	565	1.37	4.13E+03	-3.56E+03	3.56E+03	3.70E+03	7.32282E-08
D1-2B	600	2.29	4.22E+03	-3.62E+03	3.62E+03	3.72E+03	7.20795E-08

OVERALL FIT			
Multiple R	0.48542350	AIC	50.37002219
R Square	0.23563597	AICc	50.77002219
Adjusted R Square	0.21174960	BSC	51.86652975
Standard Error	2.14714554		
Observations	33		

ANOVA				Alpha	5.00E-02	
	df	*SS*	*MS*	*F*	*p-value*	*sig*
Regression	1	44.05812539	44.05813	9.55659	0.00419	yes
Residual	31	142.9172526	4.61023			
Total	32	186.975378				

	coeff	*std err*	*t stat*	*p-value*	*lower*	*upper*	*vif*
Intercept	3965.4084	1619.494361	2.45E+00	2.02E-02	6.62E+02	7.27E+03	
Ar1268 (mg/kg)	101.4284	32.8101521	3.09E+00	4.19E-03	3.45E+01	1.68E+02	1

Iteration #4

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred Y2	Residual	ABS(Res)	Pred Y2'	Weight
36	14468	55	9.54E+03	4.92E+03	4.92E+03	5.44E+03	3.38E-08
61	122400	1300	1.36E+05	-1.34E+04	1.34E+04	4.52E+04	4.90E-10
68	40850	330	3.74E+04	3.41E+03	3.41E+03	1.42E+04	4.95E-09
1718	8750	56	9.65E+03	-8.95E+02	8.95E+02	5.47E+03	3.34E-08
BR048	391	1.4	4.11E+03	-3.72E+03	3.72E+03	3.73E+03	7.20E-08
C-15	1348	0.099	3.98E+03	-2.63E+03	2.63E+03	3.69E+03	7.36E-08
C-6	44710	7.58	4.73E+03	4.00E+04	4.00E+04	3.93E+03	6.49E-08
111	5036	6.1	4.58E+03	4.52E+02	4.52E+02	3.88E+03	6.65E-08
EPA-E3	219200	3800	3.89E+05	-1.70E+05	1.70E+05	1.25E+05	6.41E-11
EPA-F2	77700	1188	1.24E+05	-4.68E+04	4.68E+04	4.16E+04	5.78E-10
EPA-H1	507600	4000	4.10E+05	9.79E+04	9.79E+04	1.31E+05	5.80E-11
GRID MARSH	3690	6.1	4.58E+03	-8.94E+02	8.94E+02	3.88E+03	6.65E-08
117	148	11	5.08E+03	-4.93E+03	4.93E+03	4.03E+03	6.14E-08
110	630	0.25	3.99E+03	-3.36E+03	3.36E+03	3.69E+03	7.34E-08
100	71	1.1	4.08E+03	-4.01E+03	4.01E+03	3.72E+03	7.23E-08
101	161	0.085	3.97E+03	-3.81E+03	3.81E+03	3.69E+03	7.36E-08
102	147	0.13	3.98E+03	-3.83E+03	3.83E+03	3.69E+03	7.35E-08
D2-1A	3831	3.03	4.27E+03	-4.42E+02	4.42E+02	3.78E+03	7.00E-08
D2-1B	3162	3.22	4.29E+03	-1.13E+03	1.13E+03	3.79E+03	6.98E-08
EC-3A	3810	24.4	6.44E+03	-2.63E+03	2.63E+03	4.46E+03	5.02E-08
EC-3B	20737	22.1	6.21E+03	1.45E+04	1.45E+04	4.39E+03	5.19E-08
EC-4A	17065	28.8	6.89E+03	1.02E+04	1.02E+04	4.60E+03	4.72E-08
EC-4B	3446	7.66	4.74E+03	-1.30E+03	1.30E+03	3.93E+03	6.48E-08
LC-1A	728	0.721	4.04E+03	-3.31E+03	3.31E+03	3.71E+03	7.28E-08
LC-1B	2958	0.964	4.06E+03	-1.11E+03	1.11E+03	3.71E+03	7.25E-08
PC-1A	13310	31.1	7.12E+03	6.19E+03	6.19E+03	4.68E+03	4.57E-08
PC-1B	4611	24.5	6.45E+03	-1.84E+03	1.84E+03	4.46E+03	5.02E-08
PC-2A	649	1.24	4.09E+03	-3.44E+03	3.44E+03	3.72E+03	7.22E-08
PC-2B	207	1.03	4.07E+03	-3.86E+03	3.86E+03	3.72E+03	7.24E-08
PC-3A	316	1.89	4.16E+03	-3.84E+03	3.84E+03	3.74E+03	7.14E-08
PC-3B	206	0.604	4.03E+03	-3.82E+03	3.82E+03	3.70E+03	7.30E-08
D1-2A	565	1.37	4.10E+03	-3.54E+03	3.54E+03	3.73E+03	7.20E-08
D1-2B	600	2.29	4.20E+03	-3.60E+03	3.60E+03	3.76E+03	7.09E-08

OVERALL FIT			
Multiple R	0.497044991	AIC	49.85406505
R Square	0.237212824	AICc	50.25406505
Adjusted R Square	0.213375724	BSC	51.35057261
Standard Error	2.130425596		
Observations	33		

ANOVA				Alpha	0.05	
	df	*SS*	*MS*	*F*	*p-value*	*sig*
Regression	1	4.38E+01	43.75515	9.640431519	0.004046	yes
Residual	31	140.7001098	4.538713			
Total	32	184.4552638				

	coeff	*std err*	*t stat*	*p-value*	*lower*	*upper*	*vif*
Intercept	**3970.027431**	**1619.841606**	2.450874	0.02009056	666.3387	7273.716	
Ar1268 (mg/kg)	**101.2668319**	**32.61512041**	3.104904	0.004046491	34.74786	167.7858	1

Case 3a: PCDD/F Concentration and Aroclor 1268 (Original Distribution)

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight	Weight * X	Weight*X^2
36	14468	55	9539.70	4928.297	4928.30	5432.161848	3.38887E-08	1.86388E-06	0.000102513
61	122400	1300	135616.91	-13216.910	13216.91	45150.49863	4.90541E-10	6.37703E-07	0.000829013
68	40850	330	37388.08	3461.917	3461.92	14205.28845	4.95564E-09	1.63536E-06	0.000539669
1718	8750	56	9640.97	-890.970	890.97	5464.064127	3.34941E-08	1.87567E-06	0.000105038
BR048	391	1.4	4111.80	-3720.801	3720.80	3722.199719	7.21773E-08	1.01048E-07	1.41468E-07
C-15	1348	0.099	3980.05	-2632.053	2632.05	3680.694854	7.38143E-08	7.30761E-09	7.23454E-10
C-6	44710	7.58	4737.63	39972.370	39972.37	3919.3558	6.50984E-08	4.93446E-07	3.74032E-06
111	5036	6.1	4587.76	448.326	448.33	3872.140428	6.66957E-08	4.06844E-07	2.48175E-06
EPA-E3	219200	3800	388783.99	-169583.988	169583.99	124906.195	6.40962E-11	2.43565E-07	0.000925549
EPA-F2	77700	1188	124275.02	-46575.024	46575.02	41577.44344	5.78475E-10	6.87228E-07	0.000816427
EPA-H1	507600	4000	409037.35	98562.645	98562.65	131286.6507	5.80175E-11	2.3207E-07	0.00092828
GRID MARSH	3690	6.1	4587.76	-897.755	897.76	3872.140428	6.66957E-08	4.06844E-07	2.48175E-06
117	148	11	5083.96	-4936.355	4936.35	4028.461593	6.162E-08	6.7782E-07	7.45602E-06
110	630	0.25	3995.34	-3365.344	3365.34	3685.512098	7.36214E-08	1.84054E-08	4.60134E-09
100	71	1.1	4081.42	-4010.921	4010.92	3712.629035	7.25499E-08	7.98049E-08	8.77854E-08
101	161	0.085	3978.64	-3817.536	3817.54	3680.248222	7.38322E-08	6.27574E-09	5.33438E-10
102	147	0.13	3983.19	-3835.840	3835.84	3681.683825	7.37746E-08	9.5907E-09	1.24679E-09
D2-1A	3831	3.03	4276.87	-445.866	445.87	3774.200433	7.02021E-08	2.12712E-07	6.44518E-07
D2-1B	3162	3.22	4296.11	-1134.107	1134.11	3780.261866	6.99771E-08	2.25326E-07	7.25551E-07
EC-3A	3810	24.4	6440.94	-2630.938	2630.94	4455.952125	5.03639E-08	1.22888E-06	2.99846E-05
EC-3B	20737	22.1	6208.02	14528.976	14528.98	4382.576884	5.20644E-08	1.15062E-06	2.54288E-05
EC-4A	17065	28.8	6886.51	10178.488	10178.49	4596.322151	4.73346E-08	1.36324E-06	3.92612E-05
EC-4B	3446	7.66	4745.73	-1299.731	1299.73	3921.907982	6.50137E-08	4.98005E-07	3.81472E-06
LC-1A	728	0.721	4043.04	-3314.841	3314.84	3700.538071	7.30248E-08	5.26509E-08	3.79613E-08
LC-1B	2958	0.964	4067.65	-1109.649	1109.65	3708.290325	7.27198E-08	7.01019E-08	6.75782E-08
PC-1A	13310	31.1	7119.43	6190.574	6190.57	4669.697391	4.58588E-08	1.42621E-06	4.43551E-05
PC-1B	4611	24.5	6451.06	-1840.065	1840.06	4459.142353	5.02918E-08	1.23215E-06	3.01877E-05
PC-2A	649	1.24	4095.60	-3446.298	3446.30	3717.095354	7.23757E-08	8.97458E-08	1.11285E-07
PC-2B	207	1.03	4074.33	-3867.632	3867.63	3710.395875	7.26373E-08	7.48164E-08	7.70609E-08
PC-3A	316	1.89	4161.42	-3845.222	3845.22	3737.831835	7.15749E-08	1.35276E-07	2.55673E-07
PC-3B	206	0.604	4031.19	-3824.993	3824.99	3696.805505	7.31723E-08	4.41961E-08	2.66944E-08
D1-2A	565	1.37	4108.76	-3544.263	3544.26	3721.24265	7.22144E-08	9.89338E-08	1.35539E-07
D1-2B	600	2.29	4201.93	-3601.528	3601.53	3750.592746	7.10886E-08	1.62793E-07	3.72796E-07
						SUM	1.80332E-06	1.74485E-05	0.004438372

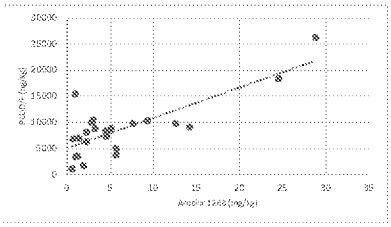
WLS Error Variance **234**

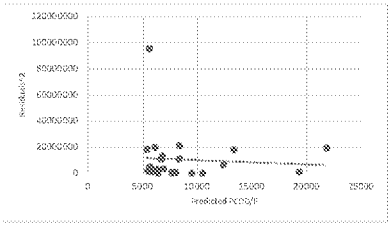
$$Var = \frac{\sum w_i}{\left((\sum w_i)(\sum w_i x_i^2) - (\sum w_i x_i)^2\right)}$$

WLS Var:OLS Var = **1.06**
Heteroscedasticity not severe

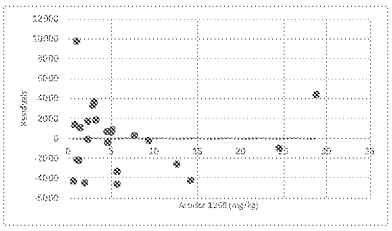
Case 1a: Furan Congener Concentration and Aroclor 1268, Excluding Outliers (Co-location Study Data)

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)	Pred PCDD/F (ng/kg)	Pred PCDD/F^2	Residual PCDD/F	Residual^2
D1-1A	8114.0	2.29	6391.43	40850321.08	1722.57	2967262.60
D1-1B	8943.5	5.12	8042.13	64675853.13	901.37	812468.08
D1-2A	6944.9	1.37	5854.80	34278693.25	1090.10	1188316.11
D1-2B	6285.4	2.29	6391.43	40850321.08	-106.03	11241.43
D2-1A	10470.6	3.03	6823.06	46554127.52	3647.54	13304558.87
D2-1B	8782.1	3.22	6933.88	48078736.04	1848.22	3415905.39
EC-1A	8337.3	4.49	7674.66	58900384.83	662.64	439093.61
EC-1B	7319.9	4.58	7727.15	59708916.81	-407.25	165856.24
EC-2A	9803.0	12.6	12405.12	153887055.90	-2602.12	6771039.75
EC-2B	3760.2	5.67	8362.94	69938734.39	-4602.74	21185198.41
EC-4A	26257.2	28.8	21854.38	477614078.61	4402.82	19384793.04
EC-4B	9798.3	7.66	9523.68	90700494.85	274.62	75415.74
LC-1A	6838.7	0.721	5476.25	29989282.64	1362.45	1856277.82
LC-1B	15393.8	0.964	5617.99	31561767.27	9775.81	95566538.37
MC-1A	10308.4	9.35	10509.44	110448266.41	-201.04	40415.88
MC-1B	10040.3	2.86	6723.90	45210825.84	3316.40	10998511.61
MC-2A	8594.3	4.98	7960.47	63369076.32	633.83	401740.97
MC-2B	9115.8	14.2	13338.38	177912448.88	-4222.58	17830203.34
MC-3A	5032.9	5.68	8368.77	70036328.39	-3335.87	11128035.47
PC-1B	18360.8	24.5	19346.25	374277243.55	-985.45	971104.29
PC-2A	3534.4	1.24	5778.97	33396534.32	-2244.57	5038110.05
PC-2B	3473.3	1.03	5656.48	31995800.40	-2183.18	4766288.19
PC-3A	1691.0	1.89	6158.11	37922324.88	-4467.11	19955076.18
PC-3B	1127.6	0.604	5408.00	29246490.67	-4280.43	18322102.09





Test for Zero Conditional Mean of Errors



No discernable relationship between residuals and independent variable
$Cov(\hat{u}_i, x_i) = 0$

Tests for Homoscedasticity

BREUSCH-PAGAN SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.072209385
R Square	0.005214195
Adjusted R Square	-0.040003341
Standard Error	19958058.24
Observations	24

$$\hat{u}^2 = d_0 + x d_1$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p>0.05
Status: Homoscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	4.59322E+13	4.59322E+13	0.115313564	0.737394415
Residual	22	8.76313E+15	3.98324E+14		
Total	23	8.80906E+15			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	11900180.61	5409827.908	2.199733672	0.038627995	680884.2063	23119477.01	680884.2063	23119477.01
Ar1268 (mg/kg)	-194508.3516	572793.4665	-0.33957851	0.737394415	-1382409.295	993392.5921	-1382409.295	993392.5921

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.252031857
R Square	0.063520057
Adjusted R Square	-0.025668509
Standard Error	19820035.55
Observations	24

$$\hat{u}^2 = d_0 + \hat{Y} \times d_1 + \hat{Y}^2 \times d_2$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p>0.05
Status: Homoscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	2	5.59552E+14	2.79776E+14	0.712199555	0.502035056
Residual	21	8.24951E+15	3.92834E+14		
Total	23	8.80906E+15			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	44901874.2	28949663.02	1.551032707	0.13583456	-15302245.82	105105994.2	-15302245.82	105105994.2
Pred PCDD/F (ng/kg)	-6507.035708	5486.446568	-1.186020064	0.248860625	-17916.72595	4902.654533	-17916.72595	4902.654533
Pred PCDD/F^2	0.240634362	0.210446219	1.143448255	0.265720578	-0.197012509	0.678281233	-0.197012509	0.678281233

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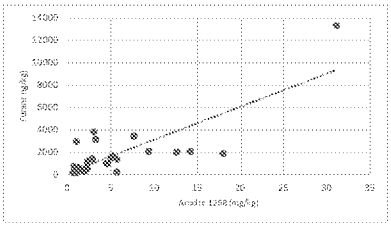
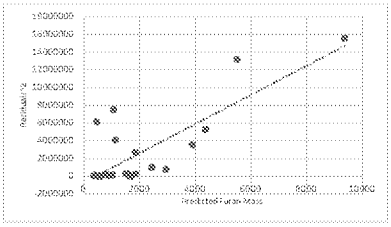
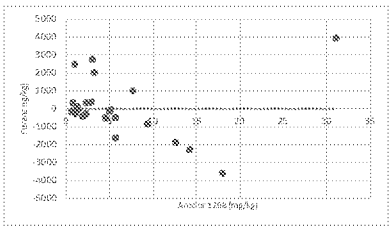
Case 1b: Furan Congener Concentration and Aroclor 1268, Excluding Outliers (Co-location Study Data)

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred PCDD/F (ng/kg)	Pred PCDD/F^2	Residual PCDD/F	Residual^2
D1-1A	1206.0	2.29	870.28	757380.79	335.72	112710.42
D1-1B	1641.0	5.12	1704.74	2906154.11	-63.74	4063.37
D1-2A	564.5	1.37	599.00	358801.42	-34.50	1190.27
D1-2B	600.4	2.29	870.28	757380.79	-269.88	72833.20
D2-1A	3831.0	3.03	1088.48	1184781.02	2742.52	7521435.33
D2-1B	3162.0	3.22	1144.50	1309882.18	2017.50	4070302.86
EC-1A	999.2	4.49	1518.98	2307298.89	-519.78	270170.79
EC-1B	1001.7	4.58	1545.52	2388624.09	-543.82	295737.38
EC-2A	2030.0	12.6	3910.34	15290725.74	-1880.34	3535662.56
EC-2B	229.9	5.67	1866.92	3485391.81	-1637.02	2679835.82
EC-4B	3446.0	7.66	2453.70	6020653.59	992.30	984655.29
LC-1A	728.2	0.721	407.63	166164.57	320.57	102763.28
LC-1B	2958.0	0.964	479.29	229714.22	2478.71	6144027.51
MC-1A	2089.0	9.35	2952.02	8714446.21	-863.02	744810.57
MC-1B	1409.0	2.86	1038.35	1078169.46	370.65	137381.87
MC-2A	1515.0	4.98	1663.46	2767110.71	-148.46	22041.40
MC-2B	2089.0	14.2	4382.12	19202975.39	-2293.12	5258399.18
MC-3A	1358.0	5.68	1869.87	3496410.30	-511.87	262009.93
MC-3B	1872.0	18	5502.61	30278688.84	-3630.61	13181310.52
PC-1A	13310.0	31.1	9365.34	87709605.64	3944.66	15560337.32
PC-2A	649.3	1.24	560.67	314348.48	88.63	7855.65
PC-2B	206.7	1.03	498.75	248747.78	-292.05	85290.99
PC-3A	316.2	1.89	752.33	566000.76	-436.13	190209.57
PC-3B	206.2	0.604	373.13	139228.73	-166.93	27866.85





Test for Zero Conditional Mean of Errors



No discernable relationship between residuals and independent variable
$Cov(\hat{u}_i, x_i) = 0$

Tests for Homoscedasticity

BREUSCH-PAGAN SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.796165103
R Square	0.633878871
Adjusted R Square	0.617237001
Standard Error	2642227.972
Observations	24

$$\hat{u}^2 = d_0 + x d_1$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p<0.05
Status: Heteroscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	2.65916E+14	2.65916E+14	38.0894028	3.2714E-06
Residual	22	1.5359E+14	6.98137E+12		
Total	23	4.19506E+14			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-380393.2471	718892.6532	-0.529137758	0.602008656	-1871285.359	1110498.865	-1871285.359	1110498.865
Ar1268 (mg/kg)	485737.7233	78704.53387	6.171661268	3.2714E-06	322514.5102	648960.9364	322514.5102	648960.9364

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.815094063
R Square	0.664378331
Adjusted R Square	0.632414363
Standard Error	2589313.161
Observations	24

$$\hat{u}^2 = d_0 + \hat{Y} \times d_1 + \hat{Y}^2 \times d_2$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p<0.05
Status: Heteroscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	2	2.78711E+14	1.39355E+14	20.78522672	1.05057E-05
Residual	21	1.40795E+14	6.70454E+12		
Total	23	4.19506E+14			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	389910.5307	1082050.564	0.360344094	0.722188873	-1860336.804	2640157.865	-1860336.804	2640157.865
Pred PCDD/F (ng/kg)	590.4088742	808.5613121	0.730196789	0.473337784	-1091.086425	2271.904173	-1091.086425	2271.904173
Pred PCDD/F^2	0.124786249	0.09033083	1.381435869	0.18166771	-0.063066996	0.312639493	-0.063066996	0.312639493

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y^	Weight	Weight * X	Weight*X^2
D1-1A	1206.0	2.29	870.28	335.724	335.72	646.0334516	2.39602E-06	5.48688E-06	1.2565E-05
D1-1B	1641.0	5.12	1704.74	-63.745	63.74	994.4479433	1.0112E-06	5.17733E-06	2.65079E-05
D1-2A	564.5	1.37	599.00	-34.500	34.50	532.7679632	3.52309E-06	4.82663E-06	6.61249E-06
D1-2B	600.4	2.29	870.28	-269.876	269.88	646.0334516	2.39602E-06	5.48688E-06	1.2565E-05
D2-1A	3831.0	3.03	1088.48	2742.524	2742.52	737.1383011	1.84036E-06	5.57628E-06	1.68961E-05
D2-1B	3162.0	3.22	1144.50	2017.499	2017.50	760.5300867	1.72889E-06	5.56702E-06	1.79258E-05
EC-1A	999.2	4.49	1518.98	-519.780	519.78	916.8857067	1.18951E-06	5.34092E-06	2.39807E-05
EC-1B	1001.7	4.58	1545.52	-543.817	543.82	927.9660262	1.16128E-06	5.31865E-06	2.43594E-05
EC-2A	2030.0	12.6	3910.34	-1880.336	1880.34	1915.34561	2.72587E-07	3.4346E-06	4.3276E-05
EC-2B	229.9	5.67	1866.92	-1637.020	1637.02	1062.161007	8.86379E-07	5.02577E-06	2.84961E-05
EC-4B	3446.0	7.66	2453.70	992.298	992.30	1307.159183	5.85252E-07	4.48303E-06	3.434E-05
LC-1A	728.2	0.721	407.63	320.567	320.57	452.866548	4.87595E-06	3.51556E-06	2.53472E-06
LC-1B	2958.0	0.964	479.29	2478.715	2478.71	482.7834107	4.29038E-06	4.13592E-06	3.98703E-06
MC-1A	2089.0	9.35	2952.02	-863.024	863.02	1515.222961	4.35559E-07	4.07248E-06	3.80776E-05
MC-1B	1409.0	2.86	1038.35	370.651	370.65	716.2088086	1.94949E-06	5.57554E-06	1.5946E-05
MC-2A	1515.0	4.98	1663.46	-148.463	148.46	977.2118907	1.04718E-06	5.21497E-06	2.59706E-05
MC-2B	2089.0	14.2	4382.12	-2293.120	2293.12	2112.329069	2.24118E-07	3.18248E-06	4.51912E-05
MC-3A	1358.0	5.68	1869.87	-511.869	511.87	1063.392154	8.84327E-07	5.02298E-06	2.85305E-05
MC-3B	1872.0	18	5502.61	-3630.607	3630.61	2580.164782	1.50212E-07	2.70382E-06	4.86687E-05
PC-1A	13310.0	31.1	9365.34	3944.659	3944.66	4192.966846	5.68797E-08	1.76896E-06	5.50146E-05
PC-2A	649.3	1.24	560.67	88.632	88.63	516.7630572	3.7447E-06	4.64343E-06	5.75785E-06
PC-2B	206.7	1.03	498.75	-292.046	292.05	490.9089783	4.14952E-06	4.27401E-06	4.40223E-06
PC-3A	316.2	1.89	752.33	-436.130	436.13	596.7875871	2.80776E-06	5.30667E-06	1.00296E-05
PC-3B	206.2	0.604	373.13	-166.934	166.93	438.4621326	5.20159E-06	3.14176E-06	1.89762E-06
						SUM	4.68082E-05	0.000108283	0.000533533

WLS Error Variance **3533**

$$Var = \frac{\sum w_i}{\left((\sum w_i)(\sum w_i x_i^2) - (\sum w_i x_i)^2\right)}$$

Case 1b: Furan Congener Concentration and Aroclor 1268, Excluding Outliers (Co-location Study Data)

Location	Furans (ng/kg)	Ar1268 (mg/kg)
D1-1A	1206.0	2.29
D1-1B	1641.0	5.12
D1-2A	564.5	1.37
D1-2B	600.4	2.29
D2-1A	3831.0	3.03
D2-1B	3162.0	3.22
EC-1A	999.2	4.49
EC-1B	1001.7	4.58
EC-2A	2030.0	12.6
EC-2B	229.9	5.67
EC-4B	3446.0	7.66
LC-1A	728.2	0.721
LC-1B	2958.0	0.964
MC-1A	2089.0	9.35
MC-1B	1409.0	2.86
MC-2A	1515.0	4.98
MC-2B	2089.0	14.2
MC-3A	1358.0	5.68
MC-3B	1872.0	18
PC-1A	13310.0	31.1
PC-2A	649.3	1.24
PC-2B	206.7	1.03
PC-3A	316.2	1.89
PC-3B	206.2	0.604

Weighted Least Squares performed with "Real Stats" Add-In

$$Pred\ Y_i' = Abs(Res)x + \partial_1$$

$$W_i = \frac{1}{Pred\ Y_i'^2}$$

WLS solution is asymptotic at Iteration #4.

Iteration #1

Location	Y: Furans (ng/kg)	X: Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y'	Weight
D1-1A	1206.0	2.29	8.70E+02	3.36E+02	3.36E+02	6.46E+02	2.40E-06
D1-1B	1641.0	5.12	1.70E+03	-6.37E+01	6.37E+01	9.94E+02	1.01E-06
D1-2A	564.5	1.37	5.99E+02	-3.45E+01	3.45E+01	5.33E+02	3.52E-06
D1-2B	600.4	2.29	8.70E+02	-2.70E+02	2.70E+02	6.46E+02	2.40E-06
D2-1A	3831.0	3.03	1.09E+03	2.74E+03	2.74E+03	7.37E+02	1.84E-06
D2-1B	3162.0	3.22	1.14E+03	2.02E+03	2.02E+03	7.61E+02	1.73E-06
EC-1A	999.2	4.49	1.52E+03	-5.20E+02	5.20E+02	9.17E+02	1.19E-06
EC-1B	1001.7	4.58	1.55E+03	-5.44E+02	5.44E+02	9.28E+02	1.16E-06
EC-2A	2030.0	12.6	3.91E+03	-1.88E+03	1.88E+03	1.92E+03	2.73E-07
EC-2B	229.9	5.67	1.87E+03	-1.64E+03	1.64E+03	1.06E+03	8.88E-07
EC-4B	3446.0	7.66	2.45E+03	9.92E+02	9.92E+02	1.31E+03	5.85E-07
LC-1A	728.2	0.721	4.08E+02	3.21E+02	3.21E+02	4.53E+02	4.88E-06
LC-1B	2958.0	0.964	4.79E+02	2.48E+03	2.48E+03	4.83E+02	4.29E-06
MC-1A	2089.0	9.35	2.95E+03	-8.63E+02	8.63E+02	1.52E+03	4.38E-07
MC-1B	1409.0	2.86	1.04E+03	3.71E+02	3.71E+02	7.16E+02	1.95E-06
MC-2A	1515.0	4.98	1.66E+03	-1.48E+02	1.48E+02	9.77E+02	1.05E-06
MC-2B	2089.0	14.2	4.38E+03	-2.29E+03	2.29E+03	2.11E+03	2.24E-07
MC-3A	1358.0	5.68	1.87E+03	-5.12E+02	5.12E+02	1.06E+03	8.84E-07
MC-3B	1872.0	18	5.50E+03	-3.63E+03	3.63E+03	2.58E+03	1.50E-07
PC-1A	13310.0	31.1	9.37E+03	3.94E+03	3.94E+03	4.19E+03	5.69E-08
PC-2A	649.3	1.24	5.61E+02	8.86E+01	8.86E+01	5.17E+02	3.74E-06
PC-2B	206.7	1.03	4.99E+02	-2.92E+02	2.92E+02	4.91E+02	4.15E-06
PC-3A	316.2	1.89	7.52E+02	-4.36E+02	4.36E+02	5.97E+02	2.81E-06
PC-3B	206.2	0.604	3.73E+02	-1.67E+02	1.67E+02	4.38E+02	5.20E-06

OVERALL FIT

Multiple R	0.410192621	AIC	20.34248779
R Square	0.168257986	AICc	20.91391636
Adjusted R Square	0.13209529	BSC	21.52054162
Standard Error	1.530570973		
Observations	24		

ANOVA (Alpha 0.05)

	df	SS	MS	F	p-value	sig
Regression	1	10.42597488	10.42597488	4.45050946	0.046497196	yes
Residual	22	51.53824508	2.342647504			
Total	23	61.96421996				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	732.3203125	307.1487002	2.384253334	0.026166107	95.33289532	1369.30773	
X-Ar1268 (mg/kg)	191.9261523	90.97651418	2.109623061	0.046497196	3.252409773	380.5998949	1

Iteration #2

Location	Y: Furans (ng/kg)	X: Ar1268 (mg/kg)	Pred Y2	Residual	ABS(Res)	Pred Y2'	Weight
D1-1A	1206.0	2.29	1.17E+03	3.42E+01	3.42E+01	5.42E+02	3.41E-06
D1-1B	1641.0	5.12	1.71E+03	-7.40E+01	7.40E+01	9.74E+02	1.05E-06
D1-2A	564.5	1.37	9.95E+02	-4.31E+02	4.31E+02	4.01E+02	6.21E-06
D1-2B	600.4	2.29	1.17E+03	-5.71E+02	5.71E+02	5.41E+02	3.41E-06
D2-1A	3831.0	3.03	1.31E+03	2.52E+03	2.52E+03	6.55E+02	2.33E-06
D2-1B	3162.0	3.22	1.35E+03	1.81E+03	1.81E+03	6.84E+02	2.14E-06
EC-1A	999.2	4.49	1.59E+03	-5.95E+02	5.95E+02	8.78E+02	1.30E-06
EC-1B	1001.7	4.58	1.61E+03	-6.10E+02	6.10E+02	8.91E+02	1.26E-06
EC-2A	2030.0	12.6	3.15E+03	-1.12E+03	1.12E+03	2.12E+03	2.23E-07
EC-2B	229.9	5.67	1.82E+03	-1.59E+03	1.59E+03	1.06E+03	8.94E-07
EC-4B	3446.0	7.66	2.20E+03	1.24E+03	1.24E+03	1.36E+03	5.39E-07
LC-1A	728.2	0.721	8.71E+02	-1.42E+02	1.42E+02	3.02E+02	1.10E-05
LC-1B	2958.0	0.964	9.17E+02	2.04E+03	2.04E+03	3.39E+02	8.69E-06
MC-1A	2089.0	9.35	2.52E+03	-4.38E+02	4.38E+02	1.62E+03	3.81E-07
MC-1B	1409.0	2.86	1.28E+03	1.28E+02	1.28E+02	6.29E+02	2.53E-06
MC-2A	1515.0	4.98	1.69E+03	-1.73E+02	1.73E+02	9.53E+02	1.10E-06
MC-2B	2089.0	14.2	3.46E+03	-1.37E+03	1.37E+03	2.36E+03	1.79E-07
MC-3A	1358.0	5.68	1.82E+03	-4.64E+02	4.64E+02	1.06E+03	8.91E-07
MC-3B	1872.0	18	4.19E+03	-2.31E+03	2.31E+03	2.94E+03	1.16E-07
PC-1A	13310.0	31.1	6.70E+03	6.61E+03	6.61E+03	4.94E+03	4.10E-08
PC-2A	649.3	1.24	9.70E+02	-3.21E+02	3.21E+02	3.81E+02	6.87E-06
PC-2B	206.7	1.03	9.30E+02	-7.23E+02	7.23E+02	3.49E+02	8.20E-06
PC-3A	316.2	1.89	1.10E+03	-7.79E+02	7.79E+02	4.81E+02	4.33E-06
PC-3B	206.2	0.604	8.48E+02	-6.42E+02	6.42E+02	2.84E+02	1.24E-05

OVERALL FIT

Multiple R	0.358774557	AIC	31.05271638
R Square	0.128719183	AICc	31.62414496
Adjusted R Square	0.090837408	BSC	32.23077021
Standard Error	1.913187335		
Observations	24		

ANOVA (Alpha 0.05)

	df	SS	MS	F	p-value	sig
Regression	1	11.8965983	11.8966	3.250182913	0.085132	no
Residual	22	80.52628716	3.660286			
Total	23	92.42288546				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	693.0761928	296.3625393	2.338609	0.028846537	78.4579	1307.694	
X-Ar1268 (mg/kg)	204.2889647	113.3048464	1.802826	0.085132081	-30.7109	439.2488	1

Iteration #3

Location	Y: Furans (ng/kg)	X: Ar1268 (mg/kg)	Pred Y3	Residual	ABS(Res)	Pred Y3'	Weight
D1-1A	1206.0	2.29	1.16E+03	4.51E+01	4.51E+01	5.60E+02	3.18E-06
D1-1B	1641.0	5.12	1.74E+03	-9.79E+01	9.79E+01	9.83E+02	1.04E-06
D1-2A	564.5	1.37	9.73E+02	-4.08E+02	4.08E+02	4.23E+02	5.59E-06
D1-2B	600.4	2.29	1.16E+03	-5.60E+02	5.60E+02	5.60E+02	3.18E-06
D2-1A	3831.0	3.03	1.31E+03	2.52E+03	2.52E+03	6.71E+02	2.22E-06
D2-1B	3162.0	3.22	1.35E+03	1.81E+03	1.81E+03	6.99E+02	2.05E-06
EC-1A	999.2	4.49	1.61E+03	-6.11E+02	6.11E+02	8.89E+02	1.27E-06
EC-1B	1001.7	4.58	1.63E+03	-6.27E+02	6.27E+02	9.02E+02	1.23E-06
EC-2A	2030.0	12.6	3.27E+03	-1.24E+03	1.24E+03	2.10E+03	2.27E-07
EC-2B	229.9	5.67	1.85E+03	-1.62E+03	1.62E+03	1.06E+03	8.82E-07
EC-4B	3446.0	7.66	2.26E+03	1.19E+03	1.19E+03	1.36E+03	5.39E-07
LC-1A	728.2	0.721	8.40E+02	-1.12E+02	1.12E+02	3.26E+02	9.39E-06
LC-1B	2958.0	0.964	8.90E+02	2.07E+03	2.07E+03	3.63E+02	7.61E-06
MC-1A	2089.0	9.35	2.60E+03	-5.14E+02	5.14E+02	1.61E+03	3.84E-07
MC-1B	1409.0	2.86	1.28E+03	1.32E+02	1.32E+02	6.45E+02	2.40E-06
MC-2A	1515.0	4.98	1.71E+03	-1.95E+02	1.95E+02	9.62E+02	1.08E-06
MC-2B	2089.0	14.2	3.59E+03	-1.50E+03	1.50E+03	2.34E+03	1.83E-07
MC-3A	1358.0	5.68	1.85E+03	-4.95E+02	4.95E+02	1.07E+03	8.87E-07
MC-3B	1872.0	18	4.37E+03	-2.50E+03	2.50E+03	2.90E+03	1.19E-07
PC-1A	13310.0	31.1	7.05E+03	6.26E+03	6.26E+03	4.86E+03	4.23E-08
PC-2A	649.3	1.24	9.46E+02	-2.97E+02	2.97E+02	4.04E+02	6.13E-06
PC-2B	206.7	1.03	9.03E+02	-6.97E+02	6.97E+02	3.72E+02	7.21E-06
PC-3A	316.2	1.89	1.08E+03	-7.63E+02	7.63E+02	5.01E+02	3.99E-06
PC-3B	206.2	0.604	8.16E+02	-6.10E+02	6.10E+02	3.09E+02	1.05E-05

OVERALL FIT

Multiple R	0.366343469	AIC	28.78773734
R Square	0.134207538	AICc	29.35916591
Adjusted R Square	0.096564387	BSC	29.96579117
Standard Error	1.825006502		
Observations	24		

ANOVA (Alpha 0.05)

	df	SS	MS	F	p-value	sig
Regression	1	11.35833362	11.35833362	3.41024663	0.078289075	no
Residual	22	73.27427212	3.330648733			
Total	23	84.63260573				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	701.3684057	297.986985	2.353688805	0.027934277	83.38122289	1319.355589	
X-Ar1268 (mg/kg)	201.5172637	109.1237704	1.846685309	0.078289075	-24.79158485	427.8261122	1

Iteration #4

Location	Y: Furans (ng/kg)	X: Ar1268 (mg/kg)	Pred Y4	Residual	ABS(Res)	Pred Y4'	Weight
D1-1A	1206.0	2.29	1.18E+03	4.32E+01	4.32E+01	5.56E+02	3.23E-06
D1-1B	1641.0	5.12	1.73E+03	-9.21E+01	9.21E+01	9.81E+02	1.04E-06
D1-2A	564.5	1.37	9.77E+02	-4.13E+02	4.13E+02	4.18E+02	5.72E-06
D1-2B	600.4	2.29	1.15E+03	-5.62E+02	5.62E+02	5.56E+02	3.23E-06
D2-1A	3831.0	3.03	1.31E+03	2.52E+03	2.52E+03	6.67E+02	2.25E-06
D2-1B	3162.0	3.22	1.35E+03	1.81E+03	1.81E+03	6.96E+02	2.07E-06
EC-1A	999.2	4.49	1.61E+03	-6.07E+02	6.07E+02	8.88E+02	1.27E-06
EC-1B	1001.7	4.58	1.62E+03	-6.23E+02	6.23E+02	9.00E+02	1.24E-06
EC-2A	2030.0	12.6	3.24E+03	-1.21E+03	1.21E+03	2.10E+03	2.26E-07
EC-2B	229.9	5.67	1.84E+03	-1.61E+03	1.61E+03	1.06E+03	8.85E-07
EC-4B	3446.0	7.66	2.24E+03	1.20E+03	1.20E+03	1.36E+03	5.39E-07
LC-1A	728.2	0.721	8.47E+02	-1.18E+02	1.18E+02	3.21E+02	9.72E-06
LC-1B	2958.0	0.964	8.98E+02	2.06E+03	2.06E+03	3.57E+02	7.84E-06
MC-1A	2089.0	9.35	2.59E+03	-4.97E+02	4.97E+02	1.62E+03	3.83E-07
MC-1B	1409.0	2.86	1.28E+03	1.31E+02	1.31E+02	6.42E+02	2.43E-06
MC-2A	1515.0	4.98	1.70E+03	-1.90E+02	1.90E+02	9.50E+02	1.09E-06
MC-2B	2089.0	14.2	3.56E+03	-1.47E+03	1.47E+03	2.34E+03	1.82E-07
MC-3A	1358.0	5.68	1.85E+03	-4.88E+02	4.88E+02	1.06E+03	8.82E-07
MC-3B	1872.0	18	4.33E+03	-2.46E+03	2.46E+03	2.91E+03	1.18E-07
PC-1A	13310.0	31.1	6.97E+03	6.34E+03	6.34E+03	4.88E+03	4.20E-08
PC-2A	649.3	1.24	9.51E+02	-3.02E+02	3.02E+02	3.99E+02	6.30E-06
PC-2B	206.7	1.03	9.09E+02	-7.02E+02	7.02E+02	3.67E+02	7.42E-06
PC-3A	316.2	1.89	1.08E+03	-7.66E+02	7.66E+02	4.96E+02	4.06E-06
PC-3B	206.2	0.604	8.23E+02	-6.17E+02	6.17E+02	3.03E+02	1.09E-05

OVERALL FIT

Multiple R	0.36461054	AIC	29.29892975
R Square	0.132940846	AICc	29.87035032
Adjusted R Square	0.095242622	BSC	30.47698358
Standard Error	1.844546395		
Observations	24		

ANOVA (Alpha 0.05)

	df	SS	MS	F	p-value	sig
Regression	1	11.47655542	11.47656	3.373124655	0.079818	no
Residual	22	74.85173098	3.402351			
Total	23	86.3282864				

	coeff	std err	t stat	p-value	lower	upper	vif
Intercept	**699.5572771**	297.6163148	2.350534	0.028122868	82.33882	1316.776	
X-Ar1268 (mg/kg)	**202.1123029**	110.0465812	1.836607	0.079817763	-26.1103	430.3349	1

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred Y	Residual	ABS(Res)	Pred Y	Weight	Weight * X	Weight * X^2
D1-1A	1206.0	2.29	1162.39	43.606	43.61	596.9804176	3.22344E-06	7.38169E-06	1.69041E-05
D1-1B	1641.0	5.12	1734.37	-93.372	93.37	981.0171036	1.03907E-06	5.32006E-06	2.72387E-05
D1-2A	564.5	1.37	976.45	-411.951	411.95	419.1310336	5.69246E-06	7.79869E-06	1.06842E-05
D1-2B	600.4	2.29	1162.39	-561.994	561.99	596.9804176	3.22344E-06	7.38169E-06	1.69041E-05
D2-1A	3831.0	3.03	1311.96	2519.042	2519.04	687.8592684	2.24197E-06	6.79317E-06	2.05833E-05
D2-1B	3162.0	3.22	1350.36	1811.641	1811.64	696.3281625	2.0624E-06	6.64092E-06	2.13837E-05
EC-1A	999.2	4.49	1607.04	-607.842	607.84	886.6202442	1.27211E-06	5.71177E-06	2.56459E-05
EC-1B	1001.7	4.58	1625.23	-623.532	623.53	900.1055098	1.23428E-06	5.653E-06	2.58907E-05
EC-2A	2030.0	12.6	3246.17	-1216.172	1216.17	2101.792514	2.26371E-07	2.85227E-06	3.59388E-05
EC-2B	229.9	5.67	1845.53	-1615.634	1615.63	1063.42706	8.84269E-07	5.01381E-06	2.84283E-05
EC-4B	3446.0	7.66	2247.74	1198.262	1198.26	1361.801267	5.39387E-07	4.1317E-06	3.16488E-05
LC-1A	728.2	0.721	845.28	-117.080	117.08	321.8872868	9.65145E-06	6.95869E-06	5.01722E-06
LC-1B	2958.0	0.964	894.39	2063.606	2063.61	338.2975504	7.76955E-06	7.50913E-06	7.2388E-06
MC-1A	2089.0	9.35	2589.31	-500.307	500.31	1614.824588	3.83486E-07	3.58559E-06	3.35253E-05
MC-1B	1409.0	2.86	1277.60	131.402	131.40	642.3871	2.4233E-06	6.93063E-06	1.98216E-05
MC-2A	1515.0	4.98	1706.08	-191.077	191.08	960.0400238	1.08498E-06	5.4032E-06	2.69079E-05
MC-2B	2089.0	14.2	3569.55	-1480.552	1480.55	2341.53057	1.8239E-07	2.58993E-06	3.67771E-05
MC-3A	1358.0	5.68	1847.56	-489.555	489.56	1064.925423	8.81783E-07	5.00853E-06	2.84484E-05
MC-3B	1872.0	18	4337.58	-2465.579	2465.58	2910.908452	1.18017E-07	2.1243E-06	3.82374E-05
PC-1A	13310.0	31.1	6985.25	6324.750	6324.75	4873.763783	4.20989E-08	1.30928E-06	4.07185E-05
PC-2A	649.3	1.24	950.18	-300.877	300.88	399.6523198	6.26098E-06	7.76349E-06	9.62673E-06
PC-2B	206.7	1.03	907.73	-701.033	701.03	388.1869988	7.37673E-06	7.59803E-06	7.82597E-06
PC-3A	316.2	1.89	1081.55	-765.350	765.35	497.0459037	4.04769E-06	7.65013E-06	1.44587E-05
PC-3B	206.2	0.604	821.63	-615.433	615.43	304.3564415	1.07953E-05	6.52037E-06	3.9383E-06
						SUM	7.26769E-05	0.00013563	0.000533792

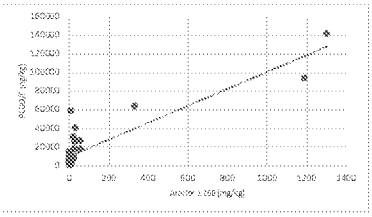
WLS Error Variance 3563

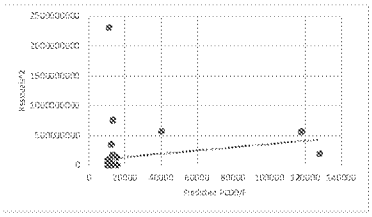
$$Var = \frac{\sum w_i}{\left((\sum w_i)(\sum w_i x_i^2) - (\sum w_i x_i)^2\right)}$$

WLS Var: OLS Var =	1.0
Heteroscedasticity not severe	

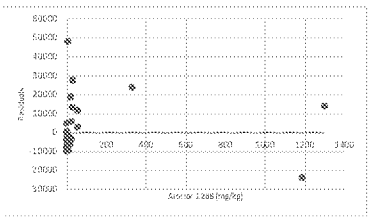
Case 2a: PCDD/F Concentration and Aroclor 1268, Excluding Outliers (Cumulative Data Set)

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)	Pred PCDD/F (ng/kg)	Pred PCDD/F^2	Residual PCDD/F	Residual^2
36	27038	55	15448.22	238647459.34	11589.68	134320710.24
61	141906	1300	128007.65	16385959692.71	13898.34	193163962.84
68	64192	330	40310.74	1624956138.98	23881.25	570314307.62
1718	18409	56	15538.63	241448954.90	2870.57	8240185.27
BR048	2981	1.4	10602.29	112408474.65	-7621.29	58084004.66
C-15	10834	0.099	10484.66	109928178.00	349.34	122035.65
C-6	59189	7.58	11161.02	124568257.20	48027.98	2306687255.47
C-8	10654	2.2	10674.61	113947376.41	-20.21	408.59
111	9396	6.1	11027.21	121599348.62	-1630.84	2659647.15
EPA-F2	94088	1188	117881.83	13896124906.83	-23794.13	566160433.26
GRID MARSH	5980	6.1	11027.21	121599348.62	-5047.21	25474324.52
117	2133	11	11470.21	131565820.13	-9336.80	87175852.47
110	3049	0.25	10498.32	110214633.17	-7449.72	55498264.46
100	856	1.1	10575.16	111834083.85	-9719.46	94467971.47
101	2058	0.085	10483.40	109901638.12	-8425.80	70994176.66
102	2678	0.13	10487.47	109986956.27	-7809.45	60987503.49
D1-1A	8114	2.29	10682.75	114121157.58	-2568.75	6598478.97
D1-1B	8944	5.12	10938.61	119653155.14	-1995.11	3980457.78
D1-2A	6945	1.37	10599.57	112350969.36	-3654.67	13356642.18
D1-2B	6285	2.29	10682.75	114121157.58	-4397.35	19336691.15
D2-1A	10471	3.03	10749.65	115555045.35	-279.05	77870.73
D2-1B	8782	3.22	10766.83	115924650.03	-1984.73	3939157.19
EC-1A	8337	4.49	10881.65	118410321.47	-2544.35	6473720.37
EC-1B	7320	4.58	10889.79	118587471.89	-3569.89	12744096.79
EC-2A	9803	12.6	11614.87	134905185.91	-1811.87	3282869.90
EC-2B	3760	5.67	10988.33	120743473.47	-7228.13	52245914.13
EC-3A	9344	24.4	12681.70	160825453.11	-3338.00	11142227.74
EC-3B	31228	22.1	12473.76	155594599.66	18754.64	351736655.16
EC-4A	26257	28.8	13079.50	171073267.44	13177.70	173651830.49
EC-4B	9798	7.66	11168.25	124729758.83	-1369.95	1876756.96
LC-1A	6839	0.721	10540.90	111110540.27	-3702.20	13706273.41
LC-1B	15394	0.964	10562.87	111574178.03	4830.93	23337905.06
MC-1A	10308	9.35	11321.04	128165931.28	-1012.64	1025438.39
MC-1B	10040	2.86	10734.28	115224846.65	-693.98	481613.38
MC-2A	8594	4.98	10925.95	119376409.15	-2331.65	5436597.22
MC-2B	9116	14.2	11759.52	138286401.66	-2643.72	6989275.90
MC-3A	5033	5.68	10989.24	120763343.21	-5956.34	35477957.71
MC-3B	6018	18	12103.08	146484515.86	-6084.78	37024532.75
PC-1A	40766	31.1	13287.44	176556038.06	27478.86	755087795.90
PC-1B	18361	24.5	12690.74	161054843.24	5670.06	32149597.61
PC-2A	3534	1.24	10587.82	112101949.80	-7053.42	49750745.32
PC-2B	3473	1.03	10568.83	111700271.04	-7095.53	50346615.45
PC-3A	1691	1.89	10646.59	113349810.38	-8955.59	80202534.84
PC-3B	1128	0.604	10530.32	110887651.56	-9402.75	88411718.50





Test for Zero Conditional Mean of Errors



No discernable relationship between residuals and independent variable
$Cov(\hat{u}_i, x_i) = 0$

Tests for Homoscedasticity

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.174021468
R Square	0.030283471
Adjusted R Square	0.007194983
Standard Error	371182846.5
Observations	44

$$\hat{u}^2 = d_0 + x d_1$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p>0.05
Status: Homoscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1.80712E+17	1.80712E+17	1.311626403	0.258584621
Residual	42	5.78662E+18	1.37777E+17		
Total	43	5.96733E+18			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	120107474.9	58109806.81	2.066905424	0.044943247	2837137	237377812.8	2837137	237377812.8
Ar1268 (mg/kg)	245964.9515	214767.2974	1.145262591	0.258584621	-187453.0017	679382.9048	-187453.0017	679382.9048

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.26801126
R Square	0.071830036
Adjusted R Square	0.026553452
Standard Error	367546228.8
Observations	44

$$\hat{u}^2 = d_0 + \hat{Y} \times d_1 + \hat{Y}^2 \times d_2$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p>0.05
Status: Homoscedastic

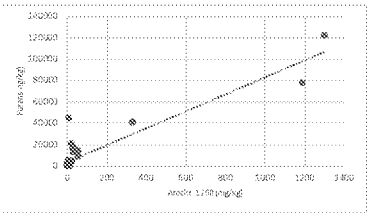
ANOVA

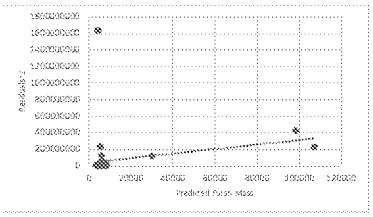
	df	*SS*	*MS*	*F*	*Significance F*
Regression	2	4.28634E+17	2.14317E+17	1.586472073	0.216952154
Residual	41	5.5387E+18	1.3509E+17		
Total	43	5.96733E+18			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-176807270.7	209618804	-0.843470468	0.403859668	-600141033.5	246526492.1	-600141033.5	246526492.1
Pred PCDD/F (ng/kg)	27879.9853	18720.20042	1.489299509	0.144061262	-9926.226419	65686.19701	-9926.226419	65686.19701
Pred PCDD/F^2	-0.190333336	0.140497673	-1.354708106	0.18292899	-0.474074142	0.09340747	-0.474074142	0.09340747

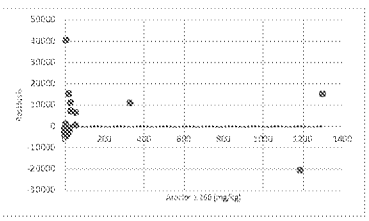
Case 2b: Furan Congener Cncentration and Aroclor 1268, Excluding Outliers (Cumulative Data Set)

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred PCDD/F (ng/kg)	Pred PCDD/F^2	Residual PCDD/F	Residual^2
36	14468	55	8046.63	64748193.11	6421.37	41234040.54
61	122400	1300	107225.33	11497271349.46	15174.67	230270580.31
68	40850	330	29953.57	897216281.25	10896.43	118732193.34
1718	8750	56	8126.29	66036553.47	623.71	389016.95
BR048	391	1.4	3776.76	14263945.82	-3385.76	11463397.41
C-15	1348	0.099	3673.12	13491841.25	-2325.12	5406202.43
C-6	44710	7.58	4269.07	18224981.55	40440.93	1635468568.49
C-8	2826	2.2	3840.49	14749388.19	-1014.49	1029196.54
111	5036	6.1	4151.17	17232241.42	884.91	783061.29
EPA-F2	77700	1188	98303.23	9663524940.08	-20603.23	424493067.91
GRID MARSH	3690	6.1	4151.17	17232241.42	-461.17	212681.07
117	148	11	4541.52	20625361.99	-4393.91	19306422.10
110	630	0.25	3685.15	13580353.25	-3055.15	9333960.37
100	71	1.1	3752.87	14083999.10	-3682.37	13559815.32
101	161	0.085	3672.01	13483649.50	-3510.91	12326488.46
102	147	0.13	3675.59	13509988.98	-3528.24	12448489.43
D1-1A	1206	2.29	3847.66	14804508.77	-2641.66	6978382.18
D1-1B	1641	5.12	4073.11	16590185.33	-2432.11	5915135.32
D1-2A	565	1.37	3774.37	14245899.75	-3209.87	10303291.65
D1-2B	600	2.29	3847.66	14804508.77	-3247.26	10544715.48
D2-1A	3831	3.03	3906.61	15261620.12	-75.61	5717.23
D2-1B	3162	3.22	3921.75	15380107.88	-759.75	577217.12
EC-1A	999	4.49	4022.92	16183871.71	-3023.72	9142872.40
EC-1B	1002	4.58	4030.09	16241608.10	-3028.39	9171132.99
EC-2A	2030	12.6	4668.97	21799317.83	-2638.97	6964183.56
EC-2B	230	5.67	4116.92	16949022.11	-3887.02	15108916.76
EC-3A	3810	24.4	5608.98	31460667.29	-1798.98	3236332.46
EC-3B	20737	22.1	5425.76	29438863.41	15311.24	234434093.37
EC-4A	17065	28.8	5959.49	35515545.26	11105.51	123332307.27
EC-4B	3446	7.66	4275.45	18279435.16	-829.45	687980.02
LC-1A	728	0.721	3722.67	13858299.49	-2994.47	8966872.75
LC-1B	2958	0.964	3742.03	14002799.55	-784.03	614705.35
MC-1A	2089	9.35	4410.07	19448750.29	-2321.07	5387383.26
MC-1B	1409	2.86	3893.07	15155993.13	-2484.07	6170603.19
MC-2A	1515	4.98	4061.95	16499458.08	-2546.95	6486967.02
MC-2B	2089	14.2	4796.43	23005765.05	-2707.43	7330190.93
MC-3A	1358	5.68	4117.72	16955581.95	-2759.72	7616030.32
MC-3B	1872	18	5099.15	26001296.55	-3227.15	10414475.50
PC-1A	13310	31.1	6142.71	37732931.99	7167.29	51369992.45
PC-1B	4611	24.5	5616.95	31550094.84	-1005.95	1011929.59
PC-2A	649	1.24	3764.02	14167832.09	-3114.72	9701468.70
PC-2B	207	1.03	3747.29	14042175.89	-3540.59	12535771.45
PC-3A	316	1.89	3815.80	14560315.32	-3499.60	12247187.03
PC-3B	206	0.604	3713.35	13788992.69	-3507.15	12300124.23





Test for Zero Conditional Mean of Errors



No discernable relationship between residuals and independent variable
$Cov(\hat{u}_i, x_i) = 0$

Tests for Homoscedasticity

BREUSCH-PAGAN SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.222572919
R Square	0.049538704
Adjusted R Square	0.026908673
Standard Error	250707407.7
Observations	44

$$\hat{u}^2 = d_0 + x d_1$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p>0.05
Status: Homoscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1.37592E+17	1.37592E+17	2.189069229	0.146455485
Residual	42	2.63988E+18	6.28542E+16		
Total	43	2.77747E+18			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	55366328.76	39249009.38	1.410642705	0.165714062	-23841378.93	134574036.5	-23841378.93	134574036.5
Ar1268 (mg/kg)	214623.4484	145059.9156	1.479550347	0.146455485	-78119.31305	507366.2099	-78119.31305	507366.2099

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.224546383
R Square	0.050421078
Adjusted R Square	0.004100155
Standard Error	253628584.5
Observations	44

$$\hat{u}^2 = d_0 + \hat{Y} \times d_1 + \hat{Y}^2 \times d_2$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p>0.05
Status: Homoscedastic

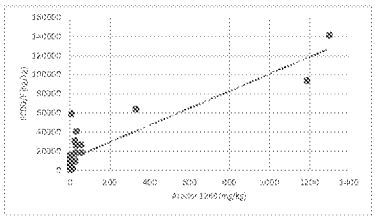
ANOVA

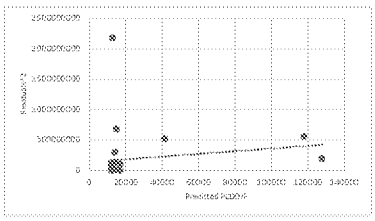
	df	*SS*	*MS*	*F*	*Significance F*
Regression	2	1.40043E+17	7.00215E+16	1.088516264	0.346247663
Residual	41	2.63743E+18	6.43275E+16		
Total	43	2.77747E+18			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	33848764	72970727.03	0.463867709	0.645195998	-113518608.9	181216136.9	-113518608.9	181216136.9
Pred PCDD/F (ng/kg)	5261.840147	13283.13063	0.396129519	0.694063569	-21563.98637	32087.66666	-21563.98637	32087.66666
Pred PCDD/F^2	-0.024374462	0.124876961	-0.195187824	0.84620999	-0.276568601	0.227819676	-0.276568601	0.227819676

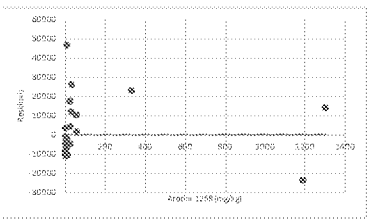
Case 3a: PCDD/F Concentration and Aroclor 1268, Excluding Outliers (Original Distribution)

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)	Pred PCDD/F (ng/kg)	Pred PCDD/F^2	Residual PCDD/F	Residual^2
36	27038	55	16744.67	280384012.67	10293.23	105950556.47
61	141906	1300	127780.77	16327926442.81	14125.22	199521946.69
68	64192	330	41270.72	1703272179.76	22921.28	525385115.12
1718	18409	56	16833.86	283378734.69	1575.34	2481706.59
BR048	2981	1.4	11964.32	143144992.42	-8983.32	80700067.65
C-15	10834	0.099	11848.29	140382003.08	-1014.29	1028786.62
C-6	59189	7.58	12515.49	156637460.17	46673.51	2178416567.24
111	9396	6.1	12383.49	153350925.75	-2987.13	8922928.22
EPA-F2	94088	1188	117791.98	13874951701.26	-23704.28	561893121.53
GRID MARSH	5980	6.1	12383.49	153350925.75	-6403.49	41004737.92
117	2133	11	12820.50	164365313.84	-10687.09	114213895.87
110	3049	0.25	11861.76	140701307.02	-8813.16	77671757.03
100	856	1.1	11937.57	142505480.98	-11081.87	122807753.10
101	2058	0.085	11847.04	140352417.12	-9789.45	95833302.86
102	2678	0.13	11851.06	140447525.96	-9173.04	84144642.67
D2-1A	10471	3.03	12109.69	146644693.97	-1639.09	2686629.84
D2-1B	8782	3.22	12126.64	147055385.16	-3344.54	11185944.36
EC-3A	9344	24.4	14015.59	196436791.97	-4671.89	21826565.81
EC-3B	31228	22.1	13810.46	190728918.47	17417.94	303384491.26
EC-4A	26257	28.8	14408.01	207590688.30	11849.19	140403356.17
EC-4B	9798	7.66	12522.62	156816103.35	-2724.32	7421939.41
LC-1A	6839	0.721	11903.76	141699611.78	-5065.06	25654879.46
LC-1B	15394	0.964	11925.44	142216040.78	3468.36	12029543.90
PC-1A	40766	31.1	14613.13	213543706.42	26153.17	683988054.02
PC-1B	18361	24.5	14024.51	196686869.36	4336.29	18803414.48
PC-2A	3534	1.24	11950.05	142803741.49	-8415.65	70823197.66
PC-2B	3473	1.03	11931.32	142356467.66	-8458.02	71538152.45
PC-3A	1691	1.89	12008.02	144192606.80	-10317.02	106440955.36
PC-3B	1128	0.604	11893.33	141451295.80	-10765.76	115901585.95
D1-2A	6945	1.37	11961.65	143080976.85	-5016.75	25167741.19
D1-2B	6285	2.29	12043.70	145050633.85	-5758.30	33157982.63





Test for Zero Conditional Mean of Errors



No discernable relationship between residuals and independent variable
$Cov(\hat{u}_i, x_i) = 0$

Tests for Homoscedasticity

BREUSCH-PAGAN SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.150080547
R Square	0.022524171
Adjusted R Square	-0.011181892
Standard Error	408917639.9
Observations	31

$$\hat{u}^2 = d_0 + x d_1$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p>0.05
Status: Homoscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1.11741E+17	1.11741E+17	0.668252787	0.420327161
Residual	29	4.8492E+18	1.67214E+17		
Total	30	4.96094E+18			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	169003086.7	77303783.54	2.186220117	0.03701769	10899097.13	327107076.2	10899097.13	327107076.2
Ar1268 (mg/kg)	196068.666	239848.9407	0.8174673	0.420327161	-294477.4972	686614.8292	-294477.4972	686614.8292

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.228677037
R Square	0.052293187
Adjusted R Square	-0.015400156
Standard Error	409769676.2
Observations	31

$$\hat{u}^2 = d_0 + \hat{Y} \times d_1 + \hat{Y}^2 \times d_2$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p>0.05
Status: Homoscedastic

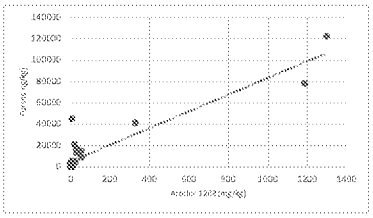
ANOVA

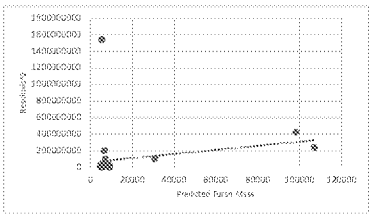
	df	*SS*	*MS*	*F*	*Significance F*
Regression	2	2.59423E+17	1.29712E+17	0.772501171	0.47145043
Residual	28	4.70151E+18	1.67911E+17		
Total	30	4.96094E+18			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-101048245.6	276161511.7	-0.36590271	0.717187736	-666739458.6	464642967.3	-666739458.6	464642967.3
Pred PCDD/F (ng/kg)	22545.33849	21862.45551	1.03123542	0.31125627	-22237.87152	67328.5485	-22237.87152	67328.5485
Pred PCDD/F^2	-0.152167302	0.162254624	-0.937830299	0.356351349	-0.484530832	0.180196228	-0.484530832	0.180196228

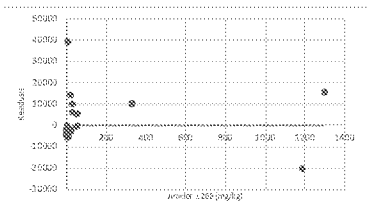
Case 3b: Furan Congener Concentration and Aroclor 1268, Excluding Outliers (Original Distribution)

Location	Furans (ng/kg)	Ar1268 (mg/kg)	Pred PCDD/F (ng/kg)	Pred PCDD/F^2	Residual PCDD/F	Residual^2
36	14468	55	9217.10	84954884.02	5250.90	27571977.55
61	122400	1300	107010.60	11451268613.06	15389.40	236833581.83
68	40850	330	30818.07	949753558.99	10031.93	100639561.43
1718	8750	56	9295.65	86409041.50	-545.65	297729.92
BR048	391	1.4	5006.87	25068757.78	-4615.87	21306265.60
C-15	1348	0.099	4904.68	24055874.23	-3556.68	12649964.12
C-6	44710	7.58	5492.30	30165401.78	39217.70	1538027656.97
111	5036	6.1	5376.05	28901928.12	-339.97	115579.84
EPA-F2	77700	1188	98213.11	9645815494.80	-20513.11	420787790.26
GRID MARSH	3690	6.1	5376.05	28901928.12	-1686.05	2842769.41
117	148	11	5760.94	33188446.30	-5613.33	31509512.34
110	630	0.25	4916.54	24172362.71	-4286.54	18374422.68
100	71	1.1	4983.31	24833342.25	-4912.81	24135666.31
101	161	0.085	4903.58	24045088.23	-4742.48	22491117.73
102	147	0.13	4907.11	24079766.13	-4759.76	22655332.67
D2-1A	3831	3.03	5134.91	26367258.86	-1303.91	1700170.66
D2-1B	3162	3.22	5149.83	26520751.44	-1987.83	3951469.04
EC-3A	3810	24.4	6813.50	46423755.30	-3003.50	9021000.37
EC-3B	20737	22.1	6632.84	43994504.46	14104.16	198927461.16
EC-4A	17065	28.8	7159.11	51252907.76	9905.89	98126585.07
EC-4B	3446	7.66	5498.59	30234467.66	-2052.59	4213116.63
LC-1A	728	0.721	4953.54	24537521.75	-4225.34	17853466.74
LC-1B	2958	0.964	4972.62	24726986.40	-2014.62	4058708.63
PC-1A	13310	31.1	7339.78	53872316.31	5970.22	35643570.89
PC-1B	4611	24.5	6821.35	46530855.68	-2210.35	4885660.04
PC-2A	649	1.24	4994.30	24943064.63	-4345.00	18879052.96
PC-2B	207	1.03	4977.81	24778571.77	-4771.11	22763470.86
PC-3A	316	1.89	5045.36	25455658.20	-4729.16	22364954.93
PC-3B	206	0.604	4944.35	24446557.91	-4738.15	22450028.03
D1-2A	565	1.37	5004.51	25045166.25	-4440.01	19713729.54
D1-2B	600	2.29	5076.78	25773691.78	-4476.38	20037974.91





Test for Zero Conditional Mean of Errors



No discernable relationship between residuals and independent variable
$Cov(\hat{u}_i, x_i) = 0$

Tests for Homoscedasticity

BREUSCH-PAGAN SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.214209487
R Square	0.045885704
Adjusted R Square	0.012985211
Standard Error	279788694.1
Observations	31

$$\hat{u}^2 = d_0 + x d_1$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p>0.05
Status: Homoscedastic

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1.09178E+17	1.09178E+17	1.394681365	0.247211408
Residual	29	2.27017E+18	7.82817E+16		
Total	30	2.37935E+18			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	76793059.1	52892618.3	1.451867228	0.157272254	-31384491.7	184970609.9	-31384491.7	184970609.9
Ar1268 (mg/kg)	193807.0716	164108.8947	1.180966285	0.247211408	-141833.3043	529447.4475	-141833.3043	529447.4475

WHITE'S SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.214211012
R Square	0.045886358
Adjusted R Square	-0.022264617
Standard Error	284740993.4
Observations	31

$$\hat{u}^2 = d_0 + \hat{Y} \times d_1 + \hat{Y}^2 \times d_2$$

H_0 = homoscedasticity of residuals
H_A = heteroscedasticity of residuals
p>0.05
Status: Homoscedastic

ANOVA

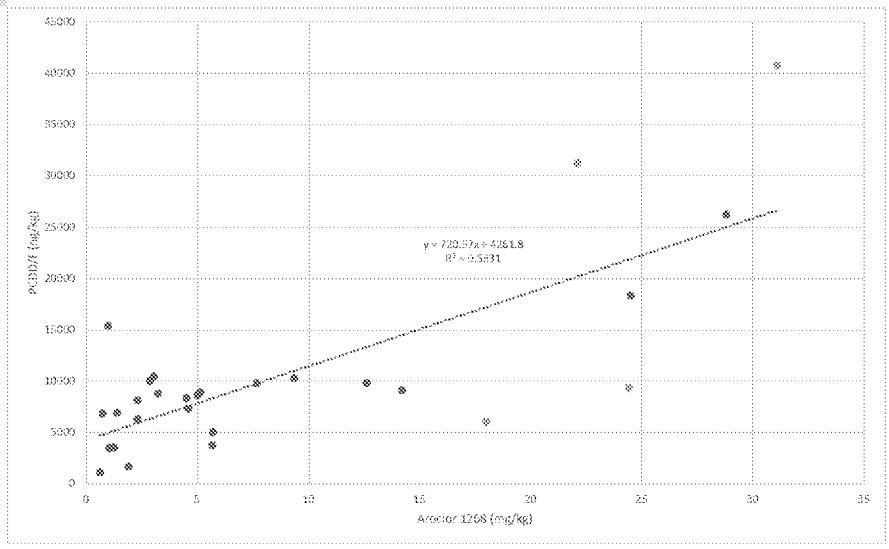
	df	*SS*	*MS*	*F*	*Significance F*
Regression	2	1.0918E+17	5.45898E+16	0.673304498	0.518085549
Residual	28	2.27017E+18	8.10774E+16		
Total	30	2.37935E+18			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	65107352.93	107523714.5	0.605516218	0.549713103	-155144991.8	285359697.7	-155144991.8	285359697.7
Pred PCDD/F (ng/kg)	2399.432246	15654.76226	0.153271714	0.879283284	-29667.89456	34466.75905	-29667.89456	34466.75905
Pred PCDD/F^2	0.000636401	0.145350216	0.004378394	0.996537604	-0.29710002	0.298372821	-0.29710002	0.298372821

APPENDIX C
Cook's Distance Calculations for Co-location Cases 1-3

Case 1a: Co-Location of PCDD/F Concentration and Aroclor 1268 (Co-location Study Data)

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)
D1-1A	8114.0	2.29
D1-1B	8943.5	5.12
D1-2A	6944.9	1.37
D1-2B	6285.4	2.29
D2-1A	10470.6	3.03
D2-1B	8782.1	3.22
EC-1A	8337.3	4.49
EC-1B	7319.9	4.58
EC-2A	9803.0	12.6
EC-2B	3760.2	5.67
EC-3A	9343.7	24.4
EC-3B	31228.4	22.1
EC-4A	26257.2	28.8
EC-4B	9798.3	7.66
LC-1A	6838.7	0.721
LC-1B	15393.8	0.964
MC-1A	10308.4	9.35
MC-1B	10040.3	2.86
MC-2A	8594.3	4.98
MC-2B	9115.8	14.2
MC-3A	5032.9	5.68
MC-3B	6018.3	18
PC-1A	40766.3	31.1
PC-1B	18360.8	24.5
PC-2A	3534.4	1.24
PC-2B	3473.3	1.03
PC-3A	1691.0	1.89
PC-3B	1127.6	0.604



Regression Analysis

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.763633914
R Square	0.583136754
Adjusted R Square	0.567103553
Standard Error	5824.838767
Observations	28

	Mean	Stnd Dev (s)	Residual Stnd Dev ($s_{\varepsilon,adj}$)
PCDD/F	10560	8853	
Ar1268	8.7	9.4	5824.8

DFFITS cutoff	0.69
D_i cutoff	0.14
p (# parameters)	2

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1234007999	1234007999	36.37057423	2.27411E-06
Residual	26	882147413.2	33928746.66		
Total	27	2116155412			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	4261.848447	1517.373234	2.80870148	0.009314981	1142.843096	7380.853798	1142.843096	7380.853798
Ar1268 (mg/kg)	720.5742178	119.4823181	6.030802122	2.27411E-06	474.9747954	966.1736401	474.9747954	966.1736401

Cooks Distance

Location	Ar1268 (mg/kg)	PCDD/F (ng/kg)	Residual (ε_i)	Leverage (h_{ii})	isr_i	esr_i	Cook's Dist (D_i)	$DFFITS_i$
D1-1A	2.29	8114.0	2202.036594	0.053222839	0.388523003	0.382088925	0.0042428	0.0905919
D1-1B	5.12	8943.5	992.311558	0.041230224	0.173983064	0.170703829	0.0006509	0.0353992
D1-2A	1.37	6944.9	1695.864875	0.058573137	0.300064103	0.294747862	0.0028010	0.0735202
D1-2B	2.29	6285.4	373.4365943	0.053222839	0.065888418	0.064614304	0.0001220	0.0153198
D2-1A	3.03	10470.6	4025.411673	0.049436206	0.708819667	0.70186943	0.0130649	0.1600620
D2-1B	3.22	8782.1	2200.002572	0.048538312	0.387207381	0.380787572	0.0038243	0.0860061
EC-1A	4.49	8337.3	840.0733152	0.043316778	0.147451503	0.144648586	0.0004922	0.0307793
EC-1B	4.58	7319.9	-242.1783644	0.04299825	-0.042500601	-0.041676715	0.0000406	-0.0088341
EC-2A	12.6	9803.0	-3538.083591	0.04198131	-0.620579164	-0.613085463	0.0084381	-0.1283400
EC-2B	5.67	3760.2	-4587.304262	0.039681706	-0.803648312	-0.798015853	0.0133437	-0.1622180
EC-3A	24.4	9343.7	12500.15856	0.138891666	2.31261211	2.544447996	0.4313152	1.0218876
EC-3B	22.1	31228.4	11061.86134	0.118088606	2.010298665	2.145001222	0.2518047	0.7572113
EC-4A	28.8	26257.2	1242.814081	0.205020125	0.239300821	0.234912601	0.0073841	0.1192962
EC-4B	7.66	9798.3	16.85304485	0.036205683	0.00294715	0.002889919	0.0000002	0.0005601
LC-1A	0.721	6838.7	2057.317542	0.062775881	0.364834326	0.35866875	0.0044577	0.0928257
LC-1B	0.964	15393.8	10437.31801	0.061160768	1.849308615	1.945883672	0.1113962	0.4966583
MC-1A	9.35	10308.4	-690.8173832	0.035870504	-0.120784627	-0.118472314	0.0002714	-0.0228517
MC-1B	2.86	10040.3	3717.60929	0.050265336	0.654905581	0.647551035	0.0113499	0.1489729
MC-2A	4.98	8594.3	743.9919485	0.041665038	0.130474506	0.127982685	0.0003701	0.0266857
MC-2B	14.2	9115.8	-5378.202339	0.048254842	-0.946439573	-0.944472356	0.0227078	-0.2126666
MC-3A	5.68	5032.9	-3321.810004	0.039655907	-0.581938976	-0.57439113	0.0069921	-0.1167208
MC-3B	18	6018.3	11213.88457	0.071788575	1.958244886	2.129796561	0.1544102	0.5923008
PC-1A	31.1	40766.3	14094.59339	0.246071156	2.786784995	3.263131114	1.2673613	1.8642309
PC-1B	24.5	18360.8	-3555.116783	0.140213853	-0.658225558	-0.650889215	0.0353281	-0.2628496
PC-2A	1.24	3534.4	-1620.960477	0.059386592	-0.286934609	-0.281809074	0.0025990	-0.0708098
PC-2B	1.03	3473.3	-1530.739891	0.060730677	-0.271158	-0.266269059	0.0023770	-0.0677064
PC-3A	1.89	1691.0	-3932.733719	0.055461537	-0.694705615	-0.68762671	0.0141692	-0.1666245
PC-3B	0.604	1127.6	-3569.505275	0.06357125	-0.633266844	-0.6258143	0.0136122	-0.1630566

(1) $\varepsilon_i = f(x_i) - f(x)$

(2) $h_{ii} = \frac{1}{n} + \frac{1}{n-1}\left(\frac{x_i - \mu_x}{s_x}\right)^2$

(3) $isr_i = \frac{\varepsilon_i}{s_{\varepsilon,adj}\sqrt{1-h_{ii}}}$

(4) $esr_i = isr_i\sqrt{\frac{n-p-1}{n-p-isr_i^2}}$

(5) $D_i = \frac{isr^2}{p}\left(\frac{h_{ii}}{1-h_{ii}}\right)$

(6) $DFFITS_i = esr_i\sqrt{\frac{h_{ii}}{1-h_{ii}}}$

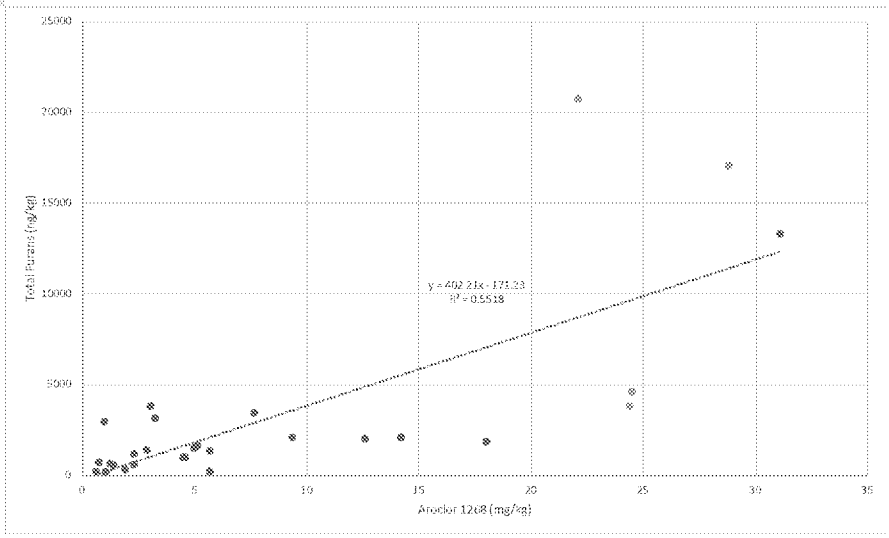
(7) $s_{\varepsilon,adj} = \sqrt{\frac{(n-1)s_\varepsilon^2}{(n-2)}}$

(8) $DFFITS\ cutoff = 2\sqrt{\frac{p+1}{n-p-1}}$

(9) $D_i cutoff = \frac{4}{n}$

Case 1b: Co-location of Furan Congener Concentration and Aroclor 1268 (Co-location Study Data)

Location	Furans (ng/kg)	Ar1268 (mg/kg)
D1-1A	1206.0	2.29
D1-1B	1641.0	5.12
D1-2A	564.5	1.37
D1-2B	600.4	2.29
D2-1A	3831.0	3.03
D2-1B	3162.0	3.22
EC-1A	999.2	4.49
EC-1B	1001.7	4.58
EC-2A	2030.0	12.6
EC-2B	229.9	5.67
EC-3A	3810.0	24.4
EC-3B	20737.0	22.1
EC-4A	17065.0	28.8
EC-4B	3446.0	7.66
LC-1A	728.2	0.721
LC-1B	2958.0	0.964
MC-1A	2089.0	9.35
MC-1B	1409.0	2.86
MC-2A	1515.0	4.98
MC-2B	2089.0	14.2
MC-3A	1358.0	5.68
MC-3B	1872.0	18
PC-1A	13310.0	31.1
PC-1B	4611.0	24.5
PC-2A	649.3	1.24
PC-2B	206.7	1.03
PC-3A	316.2	1.89
PC-3B	206.2	0.604



Regression Analysis

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.74280808
R Square	0.551763843
Adjusted R Square	0.534523991
Standard Error	3465.935399
Observations	28

	Mean	Stnd Dev (s)	Residual Stnd Dev ($s_{\varepsilon,adj}$)
PCDD/F	3344	5080	
Ar1268	8.7	9.4	3465.9
DFFITS cutoff	0.69		
D_i cutoff	0.14		
p (# parameters)	2		

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	384468380	384468380	32.00513772	5.98608E-06
Residual	26	312330413	12012708.19		
Total	27	696798793			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-171.2333681	902.8777988	-0.189652873	0.851054	-2027.125263	1684.658527	-2027.125263	1684.658527
Ar1268 (mg/kg)	402.2073895	71.09518608	5.657308346	5.98608E-06	256.0691416	548.3456375	256.0691416	548.3456375

Cooks Distance

Location	Ar1268 (mg/kg)	Furans (ng/kg)	Residual (ε_i)	Leverage (h_{ii})	isr_i	esr_i	Cook's Dist (D_i)	$DFFITS_i$
D1-1A	2.29	1206.0	456.1784461	0.053222839	0.135266549	0.13268646	0.0005143	0.0314595
D1-1B	5.12	1641.0	-247.0684663	0.041230224	-0.072801393	-0.071394916	0.0001140	-0.0148053
D1-2A	1.37	564.5	184.7092444	0.058573137	0.054925608	0.053862115	0.0000938	0.0134351
D1-2B	2.29	600.4	-149.4215539	0.053222839	-0.044306648	-0.043447883	0.0000552	-0.0103013
D2-1A	3.03	3831.0	2783.544978	0.049436206	0.823734291	0.818488841	0.0176445	0.1866572
D2-1B	3.22	3162.0	2038.125574	0.048538312	0.602857713	0.595326109	0.0092703	0.1344626
EC-1A	4.49	999.2	-635.4778109	0.043316778	-0.18745449	-0.18393859	0.0007955	-0.0391396
EC-1B	4.58	1001.7	-669.176476	0.04299825	-0.197362136	-0.193674627	0.0008751	-0.0410527
EC-2A	12.6	2030.0	-2866.57974	0.04198131	-0.844999734	-0.840207823	0.0156446	-0.1758846
EC-2B	5.67	229.9	-1879.382531	0.039681706	-0.5533337	-0.545811612	0.0063259	-0.1109508
EC-3A	24.4	3810.0	-5832.626936	0.138891866	-1.81344855	-1.90267362	0.2652277	-0.7641416
EC-3B	22.1	20737.0	12019.45006	0.110808908	3.677617503	5.206118774	0.8427160	1.8374226
EC-4A	28.8	17065.0	5652.66055	0.205020145	1.829171186	1.921345455	0.4314367	0.9758125
EC-4B	7.66	3446.0	536.3247643	0.036205683	0.157621409	0.154634407	0.0004667	0.0299711
LC-1A	0.721	728.2	609.4418402	0.062775881	0.181631042	0.17821699	0.0011048	0.0461237
LC-1B	0.964	2958.0	2741.505445	0.061160768	0.816343679	0.810951217	0.0217069	0.2069834
MC-1A	9.35	2089.0	-1500.405724	0.035870504	-0.440880168	-0.433943692	0.0036159	-0.0837017
MC-1B	2.86	1409.0	429.920234	0.050265336	0.127281791	0.124848967	0.0004287	0.0287222
MC-2A	4.98	1515.0	-316.7594318	0.041665038	-0.093357761	-0.091560164	0.0001895	-0.0190912
MC-2B	14.2	2089.0	-3451.111563	0.048254842	-1.02065319	-1.021506155	0.0264087	-0.2300123
MC-3A	5.68	1358.0	-755.3046044	0.039655907	-0.222376164	-0.218265435	0.0010210	-0.0443533
MC-3B	18	1872.0	-5196.499643	0.071788575	-1.556205634	-1.602438766	0.0936510	-0.4456415
PC-1A	31.1	13310.0	972.5835536	0.246071156	0.32317762	0.317540161	0.0170444	0.1814111
PC-1B	24.5	4611.0	-5071.847675	0.140213513	-1.578134127	-1.627419745	0.2050820	-0.6372034
PC-2A	1.24	649.3	321.7962051	0.059386592	0.095731502	0.093889009	0.0002893	0.0235914
PC-2B	1.03	206.7	-36.34024312	0.060730677	-0.010818631	-0.010608564	0.0000038	-0.0026975
PC-3A	1.89	316.2	-272.7385981	0.055461537	-0.080968541	-0.079406199	0.0001925	-0.0192416
PC-3B	0.604	206.2	134.5001048	0.06357125	0.040101885	0.03932435	0.0000546	0.0102460

(1) $\varepsilon_i = f(x_i) - f(x)$

(2) $h_{ii} = \frac{1}{n} + \frac{1}{n-1}\left(\frac{x_i - \mu_x}{s_x}\right)^2$

(3) $isr_i = \frac{\varepsilon_i}{s_{\varepsilon,adj}\sqrt{1-h_{ii}}}$

(4) $esr_i = isr_i\sqrt{\frac{n-p-1}{n-p-isr_i^2}}$

(5) $D_i = \frac{isr^2}{p}\left(\frac{h_{ii}}{1-h_{ii}}\right)$

(6) $DFFITS_i = esr_i\sqrt{\frac{h_{ii}}{1-h_{ii}}}$

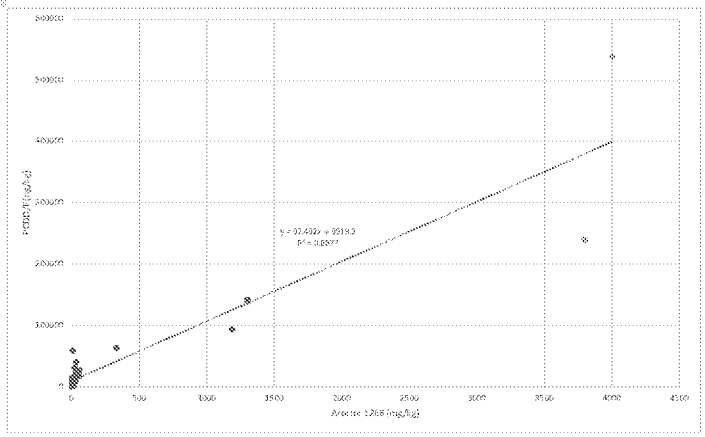
(7) $s_{\varepsilon,adj} = \sqrt{\frac{(n-1)s_\varepsilon^2}{(n-2)}}$

(8) $DFFITS\ cutoff = 2\sqrt{\frac{p+1}{n-p-1}}$

(9) $D_i cutoff = \frac{4}{n}$

Case 2a: Co-location of PCDD/F Concentration and Aroclor 1268 (Cumulative Data Set)

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)
36	27038	55
61	141906	1300
68	64192	330
1718	18409	56
BR048	2981	1.4
C-15	10834	0.099
C-6	59189	7.58
C-8	10654	2.2
111	9396	6.1
EPA-E3	240328	3800
EPA-F2	94088	1188
EPA-H1	538204	4000
GRID MARSH	5980	6.1
117	2133	11
110	3049	0.25
100	856	1.1
101	2058	0.085
102	2678	0.13
D1-1A	8114	2.29
D1-1B	8944	5.12
D1-2A	6945	1.37
D1-2B	6285	2.29
D2-1A	10471	3.03
D2-1B	8782	3.22
EC-1A	8337	4.49
EC-1B	7320	4.58
EC-2A	9803	12.6
EC-2B	3760	5.67
EC-3A	9344	24.4
EC-3B	31228	22.1
EC-4A	26257	28.8
EC-4B	9798	7.66
LC-1A	6839	0.721
LC-1B	15394	0.964
MC-1A	10308	9.35
MC-1B	10040	2.86
MC-2A	8594	4.98
MC-2B	9116	14.2
MC-3A	5033	5.68
MC-3B	6018	18
PC-1A	40766	31.1
PC-1B	18361	24.5
PC-2A	3534	1.24
PC-2B	3473	1.03
PC-3A	1691	1.89
PC-3B	1128	0.604



Regression Analysis

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.93149109
R Square	0.86767565
Adjusted R Square	0.864668279
Standard Error	31970.40714
Observations	46

	Mean	Stnd Dev (s)	Residual Stnd Dev ($s_{e,adj}$)
PCDD/F	33253	86906	
Ar1268	239.3	830.3	32331.7
DFFITS cutoff	0.53		
D_i cutoff	0.09		
p (# parameters)	2		

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	2.94894E+11	2.94894E+11	288.5162765	6.07035E-21
Residual	44	44972705045	1022106933		
Total	45	3.39867E+11			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	9919.33582	4909.876566	2.020282116	0.049467713	24.12979434	19814.54185	24.12979434	19814.54185
Ar1268 (mg/kg)	97.4922222	5.739642072	16.98576688	6.07035E-21	85.92473368	109.0597107	85.92473368	109.0597107

Cooks Distance

Location	Ar1268 (mg/kg)	PCDD/F (ng/kg)	Residual (ε_i)	Leverage (h_{ii})	isr_i	esr_i	Cook's Dist (D_i)	DFFITS$_i$
36	55	27038	11756.4918	0.022834415	0.367845611	0.364201958	0.0015810	0.0556741
61	1300	141906	5246.77403	0.05799874	0.16720087	0.165342475	0.0008606	0.0410268
68	330	64192	22100.22988	0.022004026	0.691194338	0.687034788	0.0053745	0.1030531
1718	56	18409	3030.299858	0.022822564	0.094813637	0.093739593	0.0001050	0.0143258
BR048	1.4	2981	-7074.824924	0.023563948	-0.221444913	-0.219036123	0.0005917	-0.0340265
C-15	0.099	10834	905.0124068	0.023583958	0.028327549	0.02800405	0.0000097	0.0043522
C-6	7.58	59189	48530.67228	0.023470389	1.518957118	1.542585945	0.0277266	0.2391480
C-8	2.2	10654	520.5814229	0.023551698	0.016294309	0.016108131	0.0000032	0.0025017
111	6.1	9396	-1117.671376	0.023492571	-0.034982293	-0.034582963	0.0000147	-0.0053640
EPA-E3	3800	240328	14000.13823	0.438172288	0.438278178	0.433301488	0.2485411	0.3796251
EPA-F2	1188	94088	-31652.39579	0.050745383	-1.00481739	-1.004930253	0.0269872	-0.2323501
EPA-H1	4000	538204	110435.3724	0.277968637	3.518733468	12.36928262	16.8114001	12.36928262
GRID MARSH	6.1	5980	-4534.038487	0.023492571	-0.141912072	-0.140322283	0.0002422	-0.0217648
117	11	2133	-8858.336764	0.023419671	-0.277249081	-0.274320136	0.0009217	-0.0424809
110	0.25	3049	-6895.108876	0.02358163	-0.215821681	-0.213468087	0.0005625	-0.0331743
100	1.1	856	-9170.877265	0.023568553	-0.287052885	-0.284038259	0.0009945	-0.0441288
101	0.085	2058	-7870.028659	0.023584174	-0.246337667	-0.243690386	0.0007329	-0.0378731
102	0.13	2678	-7253.992809	0.02358348	-0.227055212	-0.224591824	0.0006226	-0.0349044
D1-1A	2.29	8114	-2028.593009	0.023550323	-0.063495348	-0.062772539	0.0000486	-0.0097486
D1-1B	5.12	8944	-1474.995998	0.023507336	-0.04616664	-0.045640109	0.0000257	-0.0070813
D1-2A	1.37	6945	-3108.000165	0.023564409	-0.097281699	-0.096180216	0.0001142	-0.0149414
D1-2B	2.29	6285	-3857.193009	0.023550323	-0.120730876	-0.119370823	0.0001758	-0.0185384
D2-1A	3.03	10471	255.8627466	0.023539033	0.008008506	0.007916983	0.0000008	0.0012292
D2-1B	3.22	8782	-1451.160776	0.02353614	-0.045421279	-0.044903214	0.0000249	-0.0069714
EC-1A	4.49	8337	-2019.775898	0.023516861	-0.063218287	-0.062498607	0.0000481	-0.0096990
EC-1B	4.58	7320	-3045.950198	0.023515499	-0.095337122	-0.094257255	0.0001094	-0.0146271
EC-2A	12.6	9803	-1344.73782	0.023396203	-0.042087229	-0.041607053	0.0000212	-0.0064399
EC-2B	5.67	3760	-6711.91672	0.023499042	-0.210078756	-0.207782008	0.0005310	-0.0322327
EC-3A	24.4	9344	-2954.446042	0.023228218	-0.092459475	-0.091411642	0.0001016	-0.0140966
EC-3B	22.1	31228	19154.48607	0.023260257	0.599450033	0.5950337	0.0042787	0.0918247
EC-4A	28.8	26257	13530.08818	0.023167877	0.423411427	0.419427628	0.0021260	0.0645937
EC-4B	7.66	9798	-867.8262422	0.023469194	-0.027161998	-0.02685179	0.0000089	-0.0041627
LC-1A	0.721	6839	-3150.927712	0.023574378	-0.098625853	-0.097509442	0.0001174	-0.0151512
LC-1B	0.964	15394	5380.481678	0.023570642	0.168411854	0.166540769	0.0003423	0.0258753
MC-1A	9.35	10308	-522.4880977	0.023444046	-0.016353087	-0.016166238	0.0000032	-0.0025048
MC-1B	2.86	10040	-157.8635757	0.023541623	-0.004941138	-0.004884667	0.0000003	-0.0007584
MC-2A	4.98	8594	-1810.547087	0.02350945	-0.056669283	-0.056023657	0.0000387	-0.0086928
MC-2B	14.2	9116	-2187.925375	0.023372899	-0.06847626	-0.067697256	0.0000561	-0.0104728
MC-3A	5.68	5033	-5440.191642	0.023498891	-0.170274551	-0.168383979	0.0003489	-0.0261209
MC-3B	18	6018	-5655.89582	0.023318215	-0.17700958	-0.175048884	0.0003740	-0.0270477
PC-1A	31.1	40766	27814.95607	0.023136832	0.870429147	0.867986546	0.0089724	0.1335820
PC-1B	24.5	18361	6052.904736	0.023226833	0.189425697	0.187337163	0.0004266	0.0288883
PC-2A	1.24	3534	-6505.826176	0.023566403	-0.203635276	-0.201402866	0.0005004	-0.0312889
PC-2B	1.03	3473	-6546.452809	0.023569628	-0.204907246	-0.20266209	0.0005068	-0.0314868
PC-3A	1.89	1691	-8412.59612	0.02355644	-0.263316686	-0.260512594	0.0008364	-0.0404632
PC-3B	0.604	1128	-8850.651122	0.023576178	-0.277030734	-0.274103719	0.0009265	-0.0425924

(1) $\varepsilon_i = f(x_i) - f(\bar{x})$

(2) $h_{ii} = \frac{1}{n} + \frac{1}{n-1}\left(\frac{x_i - \mu_x}{s_x}\right)^2$

(3) $isr_i = \frac{\varepsilon_i}{s_{e,adj}\sqrt{1-h_{ii}}}$

(4) $esr_i = isr_i\sqrt{\frac{n-p-1}{n-p-isr_i^2}}$

(5) $D_i = \frac{isr^2}{p}\left(\frac{h_{ii}}{1-h_{ii}}\right)$

(6) $DFFITS_i = esr_i\sqrt{\frac{h_{ii}}{1-h_{ii}}}$

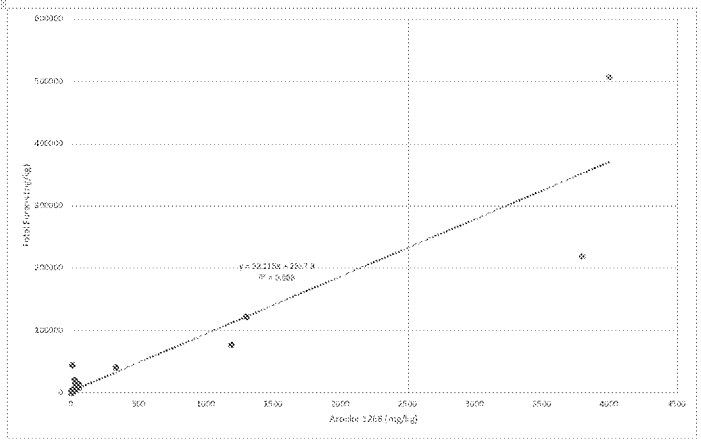
(7) $s_{e,adj} = \sqrt{\frac{(n-1)s_e^2}{(n-2)}}$

(8) $DFFITS\ cutoff = 2\sqrt{\frac{p+1}{n-p-1}}$

(9) $D_i cutoff = \frac{4}{n}$

Case 2b: Co-location of Furan Congener Concentration and Aroclor 1268 (Cumulative Data Set)

Location	Furans (ng/kg)	Ar1268 (mg/kg)
36	14468	55
61	122400	1300
68	40850	330
1718	8750	56
BR048	391	1.4
C-15	1348	0.1
C-6	44710	8
C-8	2826	2
111	5036	6
EPA-E3	219200	3800
EPA-F2	77700	1188
EPA-H1	507600	4000
GRID MARSH	3690	6
117	148	11.0
110	630	0.25
100	71	1.1
101	161	0.1
102	147	0.1
D1-1A	1206	2.3
D1-1B	1641	5.1
D1-2A	565	1.4
D1-2B	600	2.3
D2-1A	3831	3.0
D2-1B	3162	3
EC-1A	999	4.5
EC-1B	1002	4.6
EC-2A	2030	12.6
EC-2B	230	5.7
EC-3A	3810	24.4
EC-3B	20737	22
EC-4A	17065	29
EC-4B	3446	8
LC-1A	728	1
LC-1B	2958	1.0
MC-1A	2089	9
MC-1B	1409	2.9
MC-2A	1515	5.0
MC-2B	2089	14.2
MC-3A	1358	5.7
MC-3B	1872	18.0
PC-1A	13310	31.1
PC-1B	4611	25
PC-2A	649	1
PC-2B	207	1.0
PC-3A	316	1.9
PC-3B	206	0.6



Regression Analysis

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.931664686
R Square	0.867999088
Adjusted R Square	0.864999067
Standard Error	30164.6143
Observations	46

	Mean	Stnd Dev (s)	Residual Stnd Dev ($s_{\varepsilon,adj}$)
PCDD/F	24864	82097	
Ar1268	239.3	830.3	30505.5

DFFITS cutoff	0.53
D_i cutoff	0.09
p (# parameters)	2

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	2.63263E+11	2.63263E+11	289.3310295	5.75115E-21
Residual	44	40035774067	909903956.1		
Total	45	3.03299E+11			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	2817.328495	4632.550728	0.608159232	0.546208528	-6518.96403	12153.62102	-6518.96403	12153.62102
Ar1268 (mg/kg)	92.11533293	5.415448373	17.00973338	5.75115E-21	81.20121388	103.029452	81.20121388	103.029452

Cooks Distance

Location	Ar1268 (mg/kg)	Furans (ng/kg)	Residual (ε_i)	Leverage (h_{ii})	isr_i	esr_i	Cook's Dist (D_i)	$DFFITS_i$
36	55	14468	6584.328115	0.022834415	0.218348236	0.215969784	0.0005570	0.0330144
61	1300	122400	-167.2624791	0.05799874	-0.005649306	-0.005584742	0.0000010	-0.0013858
68	330	40850	7634.610696	0.022004026	0.253070002	0.250359951	0.0007205	0.0375532
1718	56	8750	774.2128979	0.022822564	0.025674145	0.025380907	0.0000077	0.0038788
BR048	1.4	391	-2555.28996	0.023563948	-0.084769689	-0.083807705	0.0000867	-0.0130193
C-15	0.1	1348	-1478.447908	0.023583958	-0.049046823	-0.048487595	0.0000291	-0.0075357
C-6	8	44710	41194.43686	0.023470389	1.366526842	1.380521713	0.0224409	0.2140231
C-8	2	2826	-193.9822459	0.023551698	-0.006435165	-0.00636162	0.0000005	-0.0009880
111	6	5036	1656.848974	0.023492571	0.054962623	0.054336324	0.0000363	0.0084279
EPA-E3	3800	219200	13[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
EPA-F2	1188	77700	-34550.34402	0.050745383	-1.162474196	-1.167252697	0.0361202	-0.2698807
EPA-H1	4000	507600	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
GRID MARSH	6	3690	310.767899	0.023492571	0.010309098	0.010191288	0.0000013	0.0015807
117	11.0	148	-3682.989157	0.023419671	-0.122171177	-0.120795379	0.0001790	-0.0187063
110	0.25	630	-2210.357328	0.02358163	-0.07332749	-0.072493864	0.0000649	-0.0112660
100	1.1	71	-2848.155361	0.023568553	-0.094485486	-0.093415094	0.0001077	-0.0145132
101	0.1	161	-2664.059298	0.023584174	-0.08837894	-0.087376617	0.0000943	-0.0135796
102	0.1	147	-2681.951488	0.02358348	-0.088972473	-0.087963525	0.0000956	-0.0136706
D1-1A	2.3	1206	-1822.272608	0.023550323	-0.060452006	-0.059763585	0.0000441	-0.0092813
D1-1B	5.1	1641	-1647.959	0.023507336	-0.05466813	-0.054045166	0.0000360	-0.0083854
D1-2A	1.4	565	-2379.026501	0.023564409	-0.078922309	-0.078025833	0.0000752	-0.0121212
D1-2B	2.3	600	-2427.872608	0.023550323	-0.080542159	-0.079627517	0.0000782	-0.0123662
D2-1A	3.0	3831	734.5620461	0.023539033	0.024368194	0.024089854	0.0000072	0.0037403
D2-1B	3	3162	48.06013283	0.02353614	0.001594334	0.001576112	0.0000000	0.0002447
EC-1A	4.5	999	-2231.72634	0.023516861	-0.074033941	-0.07319237	0.0000660	-0.0113586
EC-1B	4.6	1002	-2237.51672	0.023515499	-0.074225976	-0.073382246	0.0000663	-0.0113877
EC-2A	12.6	2030	-1947.98169	0.023396203	-0.064617176	-0.0638817	0.0000500	-0.0098876
EC-2B	5.7	230	-3109.722433	0.023499042	-0.103159112	-0.101992446	0.0001280	-0.0158218
EC-3A	24.4	3810	-1254.942619	0.023228218	-0.041624557	-0.041149642	0.0000206	-0.0063457
EC-3B	22	20737	15883.92265	0.023260257	0.526854433	0.522483703	0.0033051	0.0806289
EC-4A	29	17065	11594.74992	0.023167877	0.384568514	0.380813836	0.0017538	0.0586470
EC-4B	8	3446	-76.93194539	0.023469194	-0.002552032	-0.002522865	0.0000001	-0.0003911
LC-1A	1	728	-2155.54365	0.023574378	-0.071508809	-0.070695646	0.0000617	-0.0109848
LC-1B	1.0	2958	51.87232393	0.023570642	0.001720829	0.001701161	0.0000000	0.0002643
MC-1A	9	2089	-1589.606858	0.023444046	-0.052730691	-0.052129682	0.0000334	-0.0080771
MC-1B	2.9	1409	-1671.778347	0.023541623	-0.055459268	-0.054827343	0.0000371	-0.0085131
MC-2A	5.0	1515	-1761.062853	0.02350945	-0.058420213	-0.057754772	0.0000411	-0.0089614
MC-2B	14.2	2089	-2036.366223	0.023372899	-0.067548204	-0.066779661	0.0000546	-0.0103309
MC-3A	5.7	1358	-1982.543586	0.023498891	-0.065767098	-0.065018645	0.0000520	-0.0100861
MC-3B	18.0	1872	-2603.404488	0.023318215	-0.086354984	-0.085375273	0.0000890	-0.0131918
PC-1A	31.1	13310	7627.884651	0.023136832	0.252993611	0.250284268	0.0007580	0.0385184
PC-1B	25	4611	-463.154152	0.023226833	-0.015362115	-0.015186583	0.0000028	-0.0023418
PC-2A	1	649	-2282.251508	0.023566403	-0.075711953	-0.074851521	0.0000692	-0.0116286
PC-2B	1.0	207	-2705.507288	0.023569628	-0.089753289	-0.088735627	0.0000972	-0.0137865
PC-3A	1.9	316	-2675.226474	0.02355644	-0.088748145	-0.087741701	0.0000950	-0.0136282
PC-3B	0.6	206	-2666.766156	0.023576178	-0.088468376	-0.087465055	0.0000945	-0.0135910

(1) $\varepsilon_i = f(x_i) - f(\bar{x})$

(2) $h_{ii} = \frac{1}{n} + \frac{1}{n-1}\left(\frac{x_i - \mu_x}{s_x}\right)^2$

(3) $isr_i = \frac{\varepsilon_i}{s_{\varepsilon,adj}\sqrt{1-h_{ii}}}$

(4) $esr_i = isr_i\sqrt{\frac{n-p-1}{n-p-isr_i^2}}$

(5) $D_i = \frac{isr^2}{p}\left(\frac{h_{ii}}{1-h_{ii}}\right)$

(6) $DFFITS_i = esr_i\sqrt{\frac{h_{ii}}{1-h_{ii}}}$

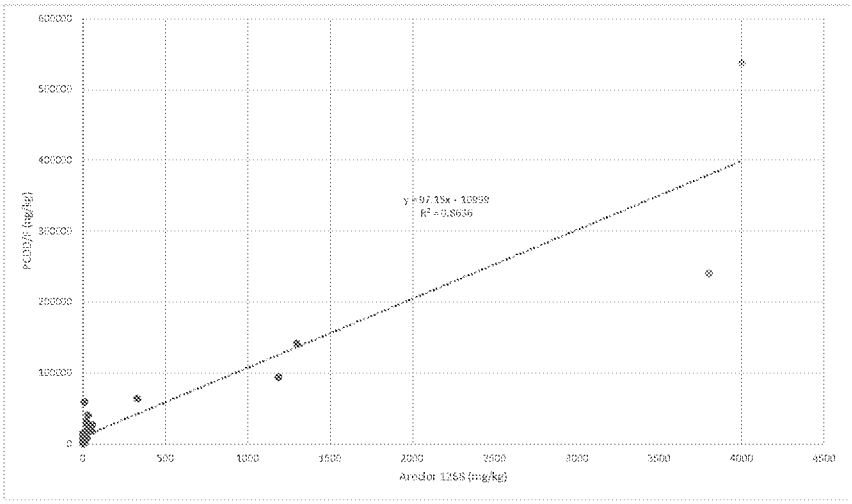
(7) $s_{\varepsilon,adj} = \sqrt{\frac{(n-1)s_\varepsilon^2}{(n-2)}}$

(8) $DFFITS\ cutoff = 2\sqrt{\frac{p+1}{n-p-1}}$

(9) $D_i cutoff = \frac{4}{n}$

Case 3a: Co-location of PCDD/F Concentration and Aroclor 1268 (Original Distribution)

Location	PCDD/F (ng/kg)	Ar1268 (mg/kg)
36	27038	55
61	141906	1300
68	64192	330
1718	18409	56
BR048	2981	1.4
C-15	10834	0.099
C-6	59189	7.58
111	9396	6.1
EPA-E3	240328	3800
EPA-F2	94088	1188
EPA-H1	538204	4000
GRID MARSH	5980	6.1
117	2133	11
110	3049	0.25
100	856	1.1
101	2058	0.085
102	2678	0.13
D2-1A	10471	3.03
D2-1B	8782	3.22
EC-3A	9344	24.4
EC-3B	31228	22.1
EC-4A	26257	28.8
EC-4B	9798	7.66
LC-1A	6839	0.721
LC-1B	15394	0.964
PC-1A	40766	31.1
PC-1B	18361	24.5
PC-2A	3534	1.24
PC-2B	3473	1.03
PC-3A	1691	1.89
PC-3B	1128	0.604
D1-2A	6945	1.37
D1-2B	6285	2.29



Regression Analysis

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.929288027
R Square	0.863576236
Adjusted R Square	0.85917547
Standard Error	38015.98318
Observations	33

	Mean	Stnd Dev (s)	Residual Stnd Dev ($s_{\varepsilon adj}$)
PCDD/F	43140	101304	
Ar1268	330.8	969.0	38016.0

DFFITS cutoff	0.63
D_i cutoff	0.12
p (# parameters)	2

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	2.83599E+11	2.83599E+11	196.2331389	5.93398E-15
Residual	31	44801664291	1445214977		
Total	32	3.28401E+11			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	10998.59331	7004.20235	1.570284918	0.126501041	-3286.571562	25283.75818	-3286.571562	25283.75818
Ar1268 (mg/kg)	97.15010107	6.935169523	14.00832391	5.93398E-15	83.00572958	111.2944726	83.00572958	111.2944726

Cooks Distance

Location	Ar1268 (mg/kg)	PCDD/F (ng/kg)	Residual (ε_i)	Leverage (h_{ii})	isr_i	esr_i	Cook's Dist (D_i)	$DFFITS_i$
36	55	27038	10696.05097	0.032835244	0.286092851	0.281812905	0.0013894	0.0519255
61	1300	141906	4612.274004	0.061561773	0.125240856	0.123235465	0.0005145	0.0315637
68	330	64192	21133.87236	0.030303054	0.564540157	0.558237012	0.0049798	0.0986833
1718	56	18409	1970.201151	0.032816917	0.052697498	0.051842893	0.0000471	0.0095496
BR048	1.4	2981	-8153.603446	0.033914948	-0.218210517	-0.214827192	0.0008358	-0.0402510
C-15	0.099	10834	-174.2112141	0.033943532	-0.00466239	-0.004586576	0.0000004	-0.0008597
C-6	7.58	59189	47454.00807	0.033780707	1.269897945	1.283066503	0.0281904	0.2399085
111	6.1	9396	-2194.841928	0.033812623	-0.058736267	-0.057784358	0.0000604	-0.0108098
EPA-E3	3800	240328	1398[illegible].7774	0.[illegible]28612	-4.[illegible]1275	-[illegible]	[illegible]	[illegible]
EPA-F2	1188	94088	-32325.21338	0.054754456	-0.874586671	-0.871179786	0.0221539	-0.2096743
EPA-H1	4000	538204	1[illegible]3.2034	0.[illegible]77	5.[illegible]3	11.[illegible]	11.[illegible]	11.[illegible]
GRID MARSH	6.1	5980	-5611.209039	0.033812623	-0.150161826	-0.147773761	0.0003946	-0.0276443
117	11	2133	-9933.830923	0.03370751	-0.265825252	-0.261801155	0.0012325	-0.0488968
110	0.25	3049	-7974.280836	0.033940208	-0.213414192	-0.210098207	0.0008001	-0.0393802
100	1.1	856	-10249.75842	0.033921529	-0.274309722	-0.270177202	0.0013210	-0.0506268
101	0.085	2058	-8949.25707	0.03394384	-0.239507749	-0.235831353	0.0010078	-0.0442060
102	0.13	2678	-8333.205824	0.033942849	-0.223020339	-0.219569966	0.0008738	-0.0411572
D2-1A	3.03	10471	-822.3581173	0.033879294	-0.022007923	-0.021650216	0.0000085	-0.0040543
D2-1B	3.22	8782	-2529.316636	0.03387515	-0.067689351	-0.066593559	0.0000803	-0.0124697
EC-3A	24.4	9344	-4025.355777	0.033428219	-0.107701311	-0.105969781	0.0002006	-0.0197070
EC-3B	22.1	31228	18082.78946	0.033475308	0.483829921	0.47776956	0.0040538	0.0889148
EC-4A	28.8	26257	12460.68378	0.033339118	0.333379258	0.328547582	0.0019166	0.0610152
EC-4B	7.66	9798	-1944.463085	0.033778985	-0.052034961	-0.051191044	0.0000473	-0.0095715
LC-1A	0.721	6839	-4229.938534	0.033929852	-0.11320445	-0.11138663	0.0002250	-0.0208747
LC-1B	0.964	15394	4301.553992	0.033924514	0.115120753	0.113272961	0.0002327	0.0212265
PC-1A	31.1	40766	26746.33855	0.033293056	0.715567639	0.709818174	0.0088172	0.1317275
PC-1B	24.5	18361	4982.029213	0.03342618	0.133297661	0.131167671	0.0003072	0.0243923
PC-2A	1.24	3534	-7584.659436	0.033918457	-0.202984542	-0.199816594	0.0007233	-0.0374406
PC-2B	1.03	3473	-7625.357915	0.033923065	-0.204074222	-0.200890707	0.0007312	-0.0376445
PC-3A	1.89	1691	-9491.207002	0.033904211	-0.254006672	-0.250136643	0.0011321	-0.0468591
PC-3B	0.604	1128	-9929.701972	0.033932423	-0.265745693	-0.26172262	0.0012403	-0.0490507
D1-2A	1.37	6945	-4186.78895	0.033915606	-0.112048826	-0.1102491	0.0002204	-0.0206570
D1-2B	2.29	6285	-4935.667042	0.033895459	-0.132089278	-0.129977924	0.0003061	-0.0243460

(1) $\varepsilon_i = f(x_i) - f(x)$

(2) $h_{ii} = \frac{1}{n} + \frac{1}{n-1}\left(\frac{x_i - \mu_x}{s_x}\right)^2$

(3) $isr_i = \frac{\varepsilon_i}{s_{\varepsilon adj}\sqrt{1-h_{ii}}}$

(4) $esr_i = isr_i\sqrt{\frac{n-p-1}{n-p-isr_i^2}}$

(5) $D_i = \frac{isr^2}{p}\left(\frac{h_{ii}}{1-h_{ii}}\right)$

(6) $DFFITS_i = esr_i\sqrt{\frac{h_{ii}}{1-h_{ii}}}$

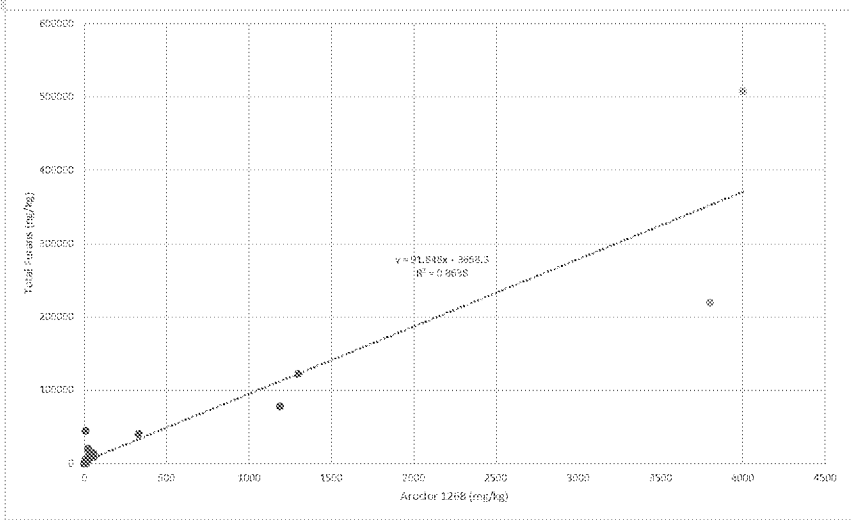
(7) $s_{\varepsilon adj} = \sqrt{\frac{(n-1)s_\varepsilon^2}{(n-2)}}$

(8) $DFFITS\ cutoff = 2\sqrt{\frac{p+1}{n-p-1}}$

(9) $D_i cutoff = \frac{4}{n}$

Case 3b: Co-location of Furan Mass and Aroclor 1268 (Original Distribution)

Location	Furans (ng/kg)	Ar1268 (mg/kg)
36	14468	55
61	122400	1300
68	40850	330
1718	8750	56
BR048	391	1.4
C-15	1348	0.1
C-6	44710	8
111	5036	6
EPA-E3	219200	3800
EPA-F2	77700	1188
EPA-H1	507600	4000
GRID MARSH	3690	6
117	148	11.0
110	630	0.25
100	71	1.1
101	161	0.1
102	147	0.1
D2-1A	3831	3.0
D2-1B	3162	3
EC-3A	3810	24.4
EC-3B	20737	22
EC-4A	17065	29
EC-4B	3446	8
LC-1A	728	1
LC-1B	2958	1.0
PC-1A	13310	31.1
PC-1B	4611	25
PC-2A	649	1
PC-2B	207	1.0
PC-3A	316	1.9
PC-3B	206	0.6
D1-2A	565	1.37
D1-2B	600	2.29



Regression Analysis

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.929419365
R Square	0.863820356
Adjusted R Square	0.859427465
Standard Error	35904.05431
Observations	33

	Mean	Stnd Dev (s)	Residual Stnd Dev ($s_{\varepsilon,adj}$)
PCDD/F	34045	95762	
Ar1268	330.8	969.0	35904.1

DFFITS cutoff	0.63
D_i cutoff	0.12
p (# parameters)	2

ANOVA

	df	SS	MS	F	Significance F
Regression	1	2.53489E+11	2.53489E+11	196.6404842	5.77075E-15
Residual	31	39962134596	1289101116		
Total	32	2.93452E+11			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	3658.299321	6615.09293	0.553023118	0.58421401	-9833.27166	17149.8703	-9833.27166	17149.8703
Ar1268 (mg/kg)	91.84823482	6.549895133	14.02285578	5.77075E-15	78.48963563	105.206834	78.48963563	105.206834

Cooks Distance

Location	Ar1268 (mg/kg)	Furans (ng/kg)	Residual (ε_i)	Leverage (h_{ii})	isr_i	esr_i	Cook's Dist (D_i)	$DFFITS_i$
36	55	14468	5758.047685	0.032835244	0.163072802	0.160489886	0.0004514	0.0295711
61	1300	122400	-661.0057633	0.061561773	-0.019004608	-0.018695678	0.0000118	-0.0047884
68	330	40850	6881.782246	0.030303054	0.194643283	0.191595253	0.0005920	0.0338696
1718	56	8750	-51.80043345	0.032816917	-0.001467018	-0.001443163	0.0000000	-0.0002658
BR048	1.4	391	-3395.886848	0.033914948	-0.096228128	-0.09467748	0.0001625	-0.0177392
C-15	0.1	1348	-2319.392291	0.033943532	-0.065724828	-0.064660566	0.0000759	-0.0121204
C-6	8	44710	40355.49064	0.033780707	1.143460816	1.149366543	0.0228563	0.2149092
111	6	5036	817.507447	0.033812623	0.023164213	0.022787731	0.0000094	0.0042629
EPA-E3	3800	219200	-13461.5817	0.430928412	-4.927888468	-10.41672243	9.1905862	-9.0610445
EPA-F2	1188	77700	-35074.00229	0.054754456	-1.004776605	-1.004937006	0.0292404	-0.2418668
EPA-H1	4000	507600	-136388.7614	0.478348877	-5.785656428	-13.94166957	13.7122502	-13.2654288
GRID MARSH	6	3690	-528.573628	0.033812623	-0.014977224	-0.014733729	0.0000039	-0.0027563
117	11.0	148	-4521.021904	0.03370751	-0.128096958	-0.126047306	0.0002862	-0.0235420
110	0.25	630	-3051.261379	0.033940208	-0.08646372	-0.08506797	0.0001313	-0.0159449
100	1.1	71	-3688.832379	0.033921529	-0.104529585	-0.102847931	0.0001918	-0.0192720
101	0.1	161	-3505.007421	0.03394384	-0.099321727	-0.097722182	0.0001733	-0.0183178
102	0.1	147	-3522.887591	0.033942849	-0.099828348	-0.098220804	0.0001751	-0.0184110
D2-1A	3.0	3831	-105.5994721	0.033879294	-0.002992282	-0.002943624	0.0000002	-0.0005512
D2-1B	3	3162	-792.0506367	0.03387515	-0.022443616	-0.022078834	0.0000088	-0.0041343
EC-3A	24.4	3810	-2089.39625	0.033428219	-0.059191625	-0.058232386	0.0000606	-0.0108294
EC-3B	22	20737	15048.85469	0.033475308	0.426337447	0.420639658	0.0031477	0.0782827
EC-4A	29	17065	10761.47152	0.033339118	0.304853437	0.300346687	0.0016026	0.0557780
EC-4B	8	3446	-915.8567993	0.033778985	-0.025950507	-0.025528796	0.0000118	-0.0047733
LC-1A	1	728	-2996.321898	0.033929852	-0.084906443	-0.083535472	0.0001266	-0.0156552
LC-1B	1.0	2958	-788.8410189	0.033924514	-0.022353239	-0.021989925	0.0000088	-0.0041207
PC-1A	31.1	13310	6795.220576	0.033293056	0.192491983	0.189475094	0.0006380	0.0351626
PC-1B	25	4611	-1297.581074	0.03342618	-0.03675983	-0.036162858	0.0000234	-0.0067249
PC-2A	1	649	-3122.891132	0.033918457	-0.088492499	-0.087064498	0.0001375	-0.0163137
PC-2B	1.0	207	-3546.203002	0.033923065	-0.10048801	-0.098870053	0.0001773	-0.0185271
PC-3A	1.9	316	-3515.692484	0.033904211	-0.099622467	-0.098018173	0.0001741	-0.0183621
PC-3B	0.6	206	-3507.575654	0.033932423	-0.099393916	-0.097793231	0.0001735	-0.0183279
D1-2A	1.37	565	-3219.631402	0.033915606	-0.091233667	-0.089762145	0.0001461	-0.0168184
D1-2B	2.29	600	-3268.231778	0.033895459	-0.092609874	-0.091116527	0.0001505	-0.0170669

(1) $\varepsilon_i = f(x_i) - f(x)$

(2) $h_{ii} = \frac{1}{n} + \frac{1}{n-1}\left(\frac{x_i - \mu_x}{s_x}\right)^2$

(3) $isr_i = \frac{\varepsilon_i}{s_{\varepsilon,adj}\sqrt{1-h_{ii}}}$

(4) $esr_i = isr_i\sqrt{\frac{n-p-1}{n-p-isr_i^2}}$

(5) $D_i = \frac{isr^2}{p}\left(\frac{h_{ii}}{1-h_{ii}}\right)$

(6) $DFFITS_i = esr_i\sqrt{\frac{h_{ii}}{1-h_{ii}}}$

(7) $s_{\varepsilon,adj} = \sqrt{\frac{(n-1)s_\varepsilon^2}{(n-2)}}$

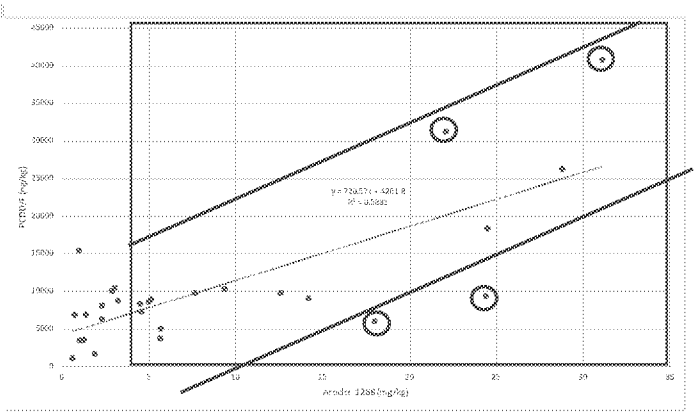
(8) $DFFITS\ cutoff = 2\sqrt{\frac{p+1}{n-p-1}}$

(9) $D_i cutoff = \frac{4}{n}$

APPENDIX D
Calculations for Co-location Cases 1-3

Case 1a: Co-location of PCDD/F Concentration and Aroclor 1268 (Co-location Study Data)

Location	Y- PCDD/F (ng/kg)	X- Ar1268 (mg/kg)
D1-1A	8114.0	2.29
D1-1B	8943.5	5.12
D1-2A	6944.9	1.37
D1-2B	6285.4	2.29
D2-1A	10470.6	3.03
D2-1B	8782.1	3.22
EC-1A	8337.3	4.49
EC-1B	7319.9	4.58
EC-2A	9803.0	12.6
EC-2B	3760.2	5.67
EC-3A	9343.7	24.4
EC-3B	31228.4	22.1
EC-4A	26257.2	28.8
EC-4B	9798.3	7.66
LC-1A	6838.7	0.721
LC-1B	15393.8	0.964
MC-1A	10308.4	9.35
MC-1B	10040.3	2.86
MC-2A	8594.3	4.98
MC-2B	9115.8	14.2
MC-3A	5032.9	5.68
MC-3B	6018.3	18
PC-1A	40766.3	31.1
PC-1B	18360.8	24.5
PC-2A	3534.4	1.24
PC-2B	3473.3	1.03
PC-3A	1691.0	1.89
PC-3B	1127.6	0.604



Regression Analysis

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.763633914
R Square	0.583136754
Adjusted R Square	0.567103553
Standard Error	5824.838767
Observations	28

H_0 = PCDD/F not correlated to Aroclor 1268
H_A = PCDD/F correlated to Aroclor 1268
$p<0.05$
Status: PCDD/F correlated to Aroclor 1268

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1234007999	1234007999	36.37057423	2.27411E-06
Residual	26	882147413.2	33928746.66		
Total	27	2116155412			

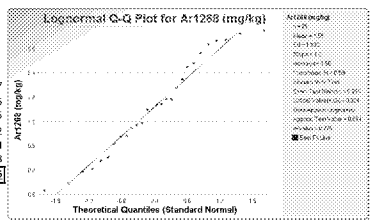
	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	4261.848447	1517.373234	2.80870148	0.009314981	1142.843096	7380.853798	1142.843096	7380.853798
Ar1268 (mg/kg)	720.5742178	119.4823181	6.030802122	2.27411E-06	474.9747954	966.1736401	474.9747954	966.1736401

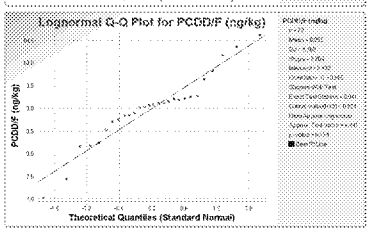
Pearson Correlation Analysis

Location	Log X	Log Y	$(\text{Log X})^2$	$(\text{Log Y})^2$	LOG X * LOG Y
D1-1A	0.4	3.9	0.129481574	15.28211831	1.406681463
D1-1B	0.7	4.0	0.503063878	15.61441161	2.802685578
D1-2A	0.1	3.8	0.018692513	14.75839763	0.525234754
D1-2B	0.4	3.8	0.129481574	14.42733298	1.366774959
D2-1A	0.5	4.0	0.231787005	16.16017141	1.935385679
D2-1B	0.5	3.9	0.257917586	15.55196817	2.002779592
EC-1A	0.7	3.9	0.425425289	15.37444041	2.557474489
EC-1B	0.7	3.9	0.43674318	14.99440004	2.553918042
EC-2A	1.1	4.0	1.210815337	15.93094669	4.391973881
EC-2B	0.8	3.6	0.567887427	12.7821333	2.6942184
EC-3A	1.4	4.0	1.92485053	15.76502022	5.508657508
EC-3B	1.3	4.5	1.807390586	20.20097731	6.042437935
EC-4A	1.5	4.4	2.129826433	19.52975653	6.449417934
EC-4B	0.9	4.0	0.781860517	15.92928417	3.529090301
LC-1A	-0.1	3.8	0.020182389	14.70702215	-0.544814503
LC-1B	0.0	4.2	0.000253541	17.53386518	-0.066674966
MC-1A	1.0	4.0	0.942475184	16.10570411	3.896052674
MC-1B	0.5	4.0	0.208269956	16.01397657	1.826261262
MC-2A	0.7	3.9	0.486128756	15.47801233	2.743047008
MC-2B	1.2	4.0	1.327768429	15.67997476	4.562825381
MC-3A	0.8	3.7	0.569041412	13.70345874	2.792460475
MC-3B	1.3	3.8	1.575709062	14.28442245	4.744269586
PC-1A	1.5	4.6	2.228333579	21.25487804	6.882075156
PC-1B	1.4	4.3	1.92978241	18.18077158	5.923253598
PC-2A	0.1	3.5	0.008727611	12.5905443	0.331489632
PC-2B	0.0	3.5	0.000164794	12.53685601	0.045453304
PC-3A	0.3	3.2	0.076431129	10.42091115	0.892458406
PC-3B	-0.2	3.1	0.047944822	9.315580021	-0.668306687

$$r = \frac{n\sum xy - (\sum x)(\sum y)}{\sqrt{[n\sum x^2 - (\sum x)^2][n\sum y^2 - (\sum y)^2]}}$$

∑LOG X	18.97144137
$\sum(\text{LOG X})^2$	19.9764365
∑LOG Y	109.3479725
$\sum(\text{LOG Y})^2$	430.0473362
∑(LOG X x Log Y)	77.12658084
n	28
r_p	0.656



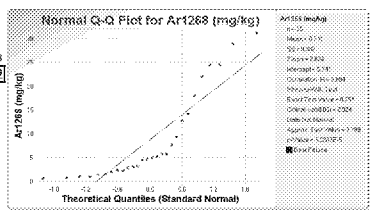


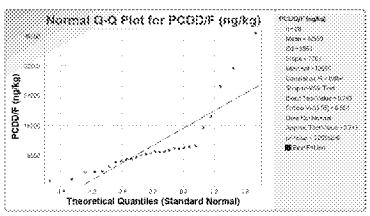
Spearman Correlation Analysis

Location	PCDD/F Rank	Ar1268 Rank	Rank Difference	Difference^2
D1-1A	17	20.5	-3.5	12.25
D1-1B	13	13	0	0
D1-2A	19	23	-4	16
D1-2B	21	20.5	0.5	0.25
D2-1A	6	18	-12	144
D2-1B	14	17	-3	9
EC-1A	16	16	0	0
EC-1B	18	15	3	9
EC-2A	9	8	1	1
EC-2B	24	12	12	144
EC-3A	11	4	7	49
EC-3B	2	5	-3	9
EC-4A	3	2	1	1
EC-4B	10	10	0	0
LC-1A	20	27	-7	49
LC-1B	5	26	-21	441
MC-1A	7	9	-2	4
MC-1B	8	19	-11	121
MC-2A	15	14	1	1
MC-2B	12	7	5	25
MC-3A	23	11	12	144
MC-3B	22	6	16	256
PC-1A	1	1	0	0
PC-1B	4	3	1	1
PC-2A	25	24	1	1
PC-2B	26	25	1	1
PC-3A	27	22	5	25
PC-3B	28	28	0	0

$$r_s = 1 - \frac{6\sum d_i^2}{n(n^2-1)}$$

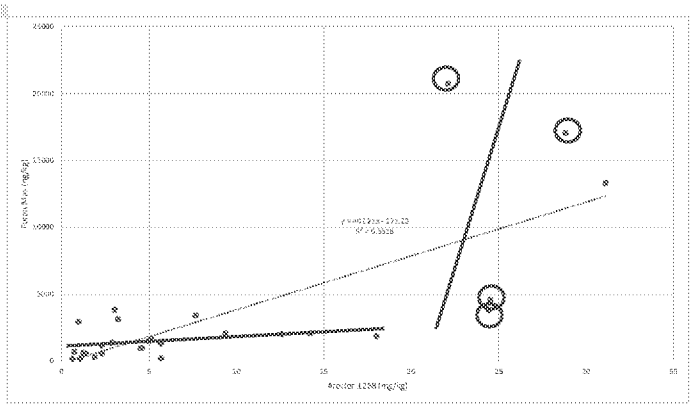
n=	28
r_s=	0.599





Case 1b: Co-location of Furan Congener Concentration and Aroclor 1268 (Co-location Study Data)

Location	Y-Furans (ng/kg)	X- Ar1268 (mg/kg)
D1-1A	1206.0	2.29
D1-1B	1641.0	5.12
D1-2A	564.5	1.37
D1-2B	600.4	2.29
D2-1A	3831.0	3.03
D2-1B	3162.0	3.22
EC-1A	999.2	4.49
EC-1B	1001.7	4.58
EC-2A	2030.0	12.5
EC-2B	229.9	5.67
EC-3A	3810.0	24.4
EC-3B	20737.0	22.1
EC-4A	17065.0	28.8
EC-4B	3446.0	7.66
LC-1A	728.2	0.721
LC-1B	2958.0	0.964
MC-1A	2089.0	9.35
MC-1B	1409.0	2.85
MC-2A	1515.0	4.98
MC-2B	2089.0	14.2
MC-3A	1358.0	5.68
MC-3B	1872.0	18
PC-1A	13310.0	31.1
PC-1B	4611.0	24.5
PC-2A	649.3	1.24
PC-2B	206.7	1.03
PC-3A	316.2	1.89
PC-3B	206.2	0.604



Regression Analysis

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.74280808
R Square	0.551763843
Adjusted R Square	0.534523991
Standard Error	3465.935399
Observations	28

H_0 = Furan mass not correlated to Aroclor 1268

H_A = Furan mass correlated to Aroclor 1268

$p<0.05$

Status: Furan mass correlated to Aroclor 1268

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	384468380	384468380	32.00513772	5.98608E-06
Residual	26	312330413	12012708.19		
Total	27	696798793			

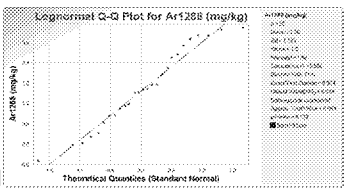
	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-171.2333681	902.8777988	-0.189652873	0.851054	-2027.125263	1684.658527	-2027.125263	1684.658527
Ar1268 (mg/kg)	402.2073895	71.09518608	5.657308346	5.98608E-06	256.0691416	548.3456375	256.0691416	548.3456375

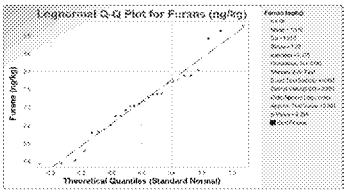
Pearson Correlation Analysis

Location	Log X	Log Y	$(\text{Log X})^2$	$(\text{Log Y})^2$	LOG X * LOG Y
D1-1A	0.4	3.1	0.129481574	9.494701231	1.108778095
D1-1B	0.7	3.2	0.503063878	10.33692319	2.280379938
D1-2A	0.1	2.8	0.018692513	7.571654473	0.376209055
D1-2B	0.4	2.8	0.129481574	7.719732632	0.999781544
D2-1A	0.5	3.6	0.231787005	12.84012598	1.725155221
D2-1B	0.5	3.5	0.257917586	12.24973306	1.777476184
EC-1A	0.7	3.0	0.425425289	8.997914673	1.956512319
EC-1B	0.7	3.0	0.43674318	9.004426587	1.983083937
EC-2A	1.1	3.3	1.210815337	10.93953004	3.639471218
EC-2B	0.8	2.4	0.567887427	5.576866313	1.779615762
EC-3A	1.4	3.6	1.92485053	12.82302368	4.96813888
EC-3B	1.3	4.3	1.807390586	18.6342954	5.803399873
EC-4A	1.5	4.2	2.129826433	17.91072367	6.176304131
EC-4B	0.9	3.5	0.781860517	12.51259934	3.127795932
LC-1A	-0.1	2.9	0.020182389	8.192478924	-0.406624884
LC-1B	0.0	3.5	0.000253541	12.04782829	-0.055268586
MC-1A	1.0	3.3	0.942475184	11.02199125	3.223034785
MC-1B	0.5	3.1	0.208269956	9.915640443	1.437056019
MC-2A	0.7	3.2	0.486128756	10.11502452	2.21747701
MC-2B	1.2	3.3	1.327768429	11.02199125	3.825526368
MC-3A	0.8	3.1	0.569041412	9.815060969	2.363297727
MC-3B	1.3	3.3	1.575709062	10.70798554	4.107635555
PC-1A	1.5	4.1	2.228333579	17.00884463	6.156409639
PC-1B	1.4	3.7	1.92978241	13.4233947	5.089619924
PC-2A	0.1	2.8	0.008727611	7.909849144	0.262743389
PC-2B	0.0	2.3	0.000164794	5.360801523	0.029722546
PC-3A	0.3	2.5	0.076431129	6.249809329	0.691143968
PC-3B	-0.2	2.3	0.047944822	5.355932006	-0.50674373

$$r = \frac{n\sum(x_i y_i) - (\sum x_i)(\sum y_i)}{\sqrt{[n\sum x_i^2 - (\sum x_i)^2][n\sum y_i^2 - (\sum y_i)^2]}}$$

$\sum$LOG X	18.97144137
$\sum(\text{LOG X})^2$	19.9764365
$\sum$LOG Y	89.68401666
$\sum(\text{LOG Y})^2$	294.7588828
$\sum$(LOG X x Log Y)	66.13713582
n	28
r_p	**0.735**



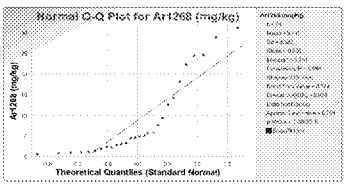


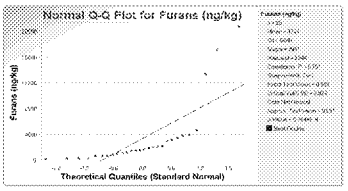
Spearman Correlation Analysis

Location	Furan Rank	Ar1268 Rank	Rank Difference	Difference^2
D1-1A	18	20.5	-2.5	6.25
D1-1B	14	13	1	1
D1-2A	24	23	1	1
D1-2B	23	20.5	2.5	6.25
D2-1A	5	18	-13	169
D2-1B	8	17	-9	81
EC-1A	20	16	4	16
EC-1B	19	15	4	16
EC-2A	12	8	4	16
EC-2B	26	12	14	196
EC-3A	6	4	2	4
EC-3B	1	5	-4	16
EC-4A	2	2	0	0
EC-4B	7	10	-3	9
LC-1A	21	27	-6	36
LC-1B	9	26	-17	289
MC-1A	10.5	9	1.5	2.25
MC-1B	16	19	-3	9
MC-2A	15	14	1	1
MC-2B	10.5	7	3.5	12.25
MC-3A	17	11	6	36
MC-3B	13	6	7	49
PC-1A	3	1	2	4
PC-1B	4	3	1	1
PC-2A	22	24	-2	4
PC-2B	27	25	2	4
PC-3A	25	22	3	9
PC-3B	28	28	0	0

$$r_s = 1 - \frac{6\sum d_i^2}{n(n^2-1)}$$

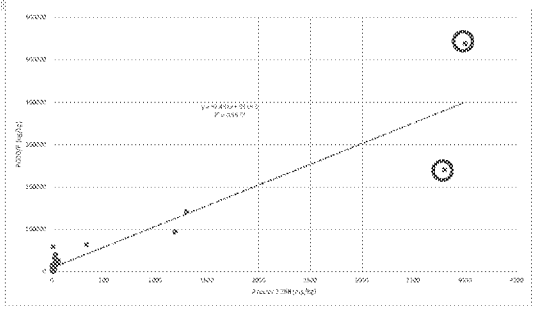
n=	28
r_s=	**0.728**





Case 2a: Co-location of PCDD/F Concentration and Aroclor 1268 (Cumulative Data Set)

Location	Y: PCDD/F (ng/kg)	X: Ar1268 (mg/kg)
36	27038	55
61	141906	1300
68	64192	350
1718	18409	56
BR048	2981	1.4
C-15	10834	0.099
C-6	59189	7.58
C-8	19654	2.2
111	9306	6.1
EPA-E3	240328	3800
EPA-F2	94088	1188
EPA-H1	558204	4690
GRID MARSH	5980	6.1
117	2158	1.1
110	3049	0.25
100	856	1.1
101	2058	0.885
102	2678	0.13
D1-1A	8114	2.29
D1-1B	8944	5.12
D1-2A	6945	1.37
D1-2B	6285	2.29
D2-1A	10471	5.03
D2-1B	8782	5.22
EC-1A	6537	4.49
EC-1B	7324	4.58
EC-2A	9803	12.6
EC-2B	3760	5.67
EC-3A	9344	24.4
EC-3B	31226	22.1
EC-4A	26257	28.8
EC-4B	9798	7.66
LC-1A	6859	0.721
LC-1B	15594	0.964
MC-1A	10368	9.35
MC-1B	10040	2.86
MC-2A	8594	4.98
MC-2B	9116	14.2
MC-3A	5033	5.68
MC-3B	5016	18
PC-1A	40766	51.1
PC-1B	18561	24.5
PC-2A	3534	1.24
PC-2B	3473	1.03
PC-3A	1691	1.89
PC-3B	1128	0.604



Regression Analysis

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.95149109
R Square	0.85767565
Adjusted R Square	0.85456279
Standard Error	31970.40714
Observations	46

H_0 = PCDD/F not correlated to Aroclor 1268
H_A = PCDD/F correlated to Aroclor 1268
p<0.05
Status: PCDD/F correlated to Aroclor 1268

ANOVA

	df	SS	MS	F	Significance F
Regression	1	2.94894E+11	2.94894E+11	288.5162765	6.07055E-21
Residual	44	44972705045	1022106933		
Total	45	3.39867E+11			

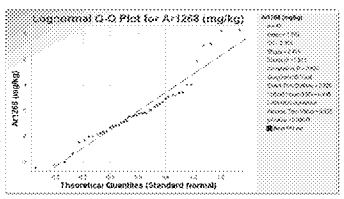
	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	9919.38582	4909.876566	2.020282115	0.048457713	24.12979434	19814.54185	24.12979434	19814.54185
Ar1268 (mg/kg)	97.4922222	5.738642072	16.98576568	6.07055E-21	85.92473368	109.0597107	85.92473368	109.0597107

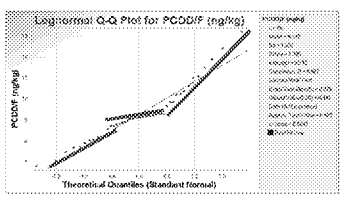
Pearson Correlation Analysis

Location	Log X	Log Y	$(\log X)^2$	$(\log Y)^2$	LOG X * LOG Y
36	1.7	4.4	3.028862291	19.64258427	7.715240572
61	3.1	5.2	9.695643201	26.54311177	15.0490585
68	2.5	4.8	6.342912455	23.11187261	12.10770766
1718	1.7	4.3	3.056161378	18.19052286	7.45602298
BR048	0.1	3.5	0.021358403	12.07119115	0.507701691
C-15	-1.0	4.0	1.008748662	16.2705209	-4.052309898
C-6	0.9	4.8	0.773817911	22.77428413	4.197993446
C-8	0.3	4.0	0.117253292	16.22008967	1.179117278
111	0.8	4.0	0.61674895	15.78441085	3.120082898
EPA-E3	3.6	5.4	12.8148506	28.95305058	19.26211552
EPA-F2	3.1	5.0	9.454496144	24.78502903	15.28270058
EPA-H1	3.6	5.7	12.97483618	32.84375446	20.6432152
GRID MARSH	0.8	3.8	0.61674895	14.26347177	2.965856111
117	1.0	3.3	1.084498725	11.08274081	3.466874594
110	-0.6	3.5	0.362476255	12.15895591	-2.097637484
100	0.0	2.9	0.001713554	8.598509567	0.121376562
101	-1.1	3.3	1.145143857	10.9783524	-3.547220171
102	-0.9	3.4	0.785995383	11.74199422	-3.037336788
D1-1A	0.4	3.9	0.129481574	15.28218381	1.406681463
D1-1B	0.7	4.0	0.503063878	15.61441161	2.802685578
D1-2A	0.1	3.8	0.018692513	14.75839763	0.525234754
D1-2B	0.4	3.8	0.129481574	14.42753196	1.166774958
D2-1A	0.5	4.0	0.231787005	16.16017141	1.935365679
D2-1B	0.5	3.9	0.257917586	15.55196817	2.002779592
EC-1A	0.7	3.9	0.425425289	15.37444041	2.557474489
EC-1B	0.7	3.9	0.43674318	14.93440004	2.558918042
EC-2A	1.1	4.0	1.210815837	15.99094669	4.391973881
EC-2B	0.8	3.6	0.567887427	12.7821338	2.6942184
EC-3A	1.4	4.0	1.92485058	15.76502022	5.508657508
EC-3B	1.3	4.5	1.807390586	20.20097731	6.042437935
EC-4A	1.5	4.4	2.138626435	19.52978653	6.648417934
EC-4B	0.9	4.0	0.781860517	15.92928417	3.529090501
LC-1A	-0.1	3.8	0.020182589	14.70702215	-0.544814503
LC-1B	0.0	4.2	0.000258541	17.55365518	-0.056674966
MC-1A	1.0	4.0	0.942475184	16.10570411	3.896052574
MC-1B	0.5	4.0	0.208269956	16.01397657	1.826361262
MC-2A	0.7	3.9	0.486128756	15.47801233	2.748047008
MC-2B	1.2	4.0	1.327768429	15.67997478	4.562825581
MC-3A	0.8	3.7	0.569041412	13.70345874	2.792460475
MC-3B	1.3	3.8	1.575709062	14.28442245	4.744269586
PC-1A	1.5	4.6	2.218353579	21.25487804	6.882075156
PC-1B	1.4	4.3	1.9278241	18.18077158	5.923255598
PC-2A	0.1	3.5	0.008727611	12.5905445	0.531489632
PC-2B	0.0	3.5	0.000164794	12.55835601	0.045453304
PC-3A	0.3	3.2	0.076451129	10.42091115	0.892458406
PC-3B	-0.2	3.1	0.047944822	9.315560021	-0.668305587

$$r = \frac{\sum(X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum(X_i - \bar{X})^2 \sum(Y_i - \bar{Y})^2}}$$

∑LOG X	38.80771185
∑(LOG X)²	83.87878646
∑LOG Y	184.6349985
∑(LOG Y)²	756.0104022
∑(LOG X x Log Y)	178.6692919
n	46
r	0.829





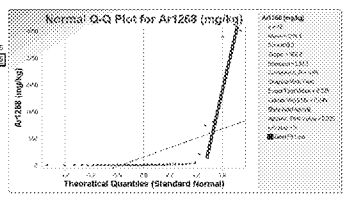
Pearson Correlation not applicable- variables do not follow normal/lognormal distribution

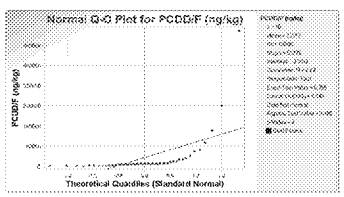
Spearman Correlation Analysis

Location	PCDD/F Rank	Ar1268 Rank	Rank Difference	Difference^2
36	9	7	2	4
61	3	3	0	0
68	5	5	0	0
1718	11	6	5	25
BR048	40	35	5	25
C-15	14	45	-31	961
C-6	6	19	-13	169
C-8	15	33	-18	324
111	21	20.5	0.5	0.25
EPA-E3	2	2	0	0
EPA-F2	4	4	0	0
EPA-H1	1	1	0	0
GRID MARSH	34	20.5	13.5	182.25
117	42	16	26	676
110	38	43	-4	16
100	46	38	8	64
101	43	46	-3	9
102	41	44	-3	9
D1-1A	26	31.5	-5.5	12.25
D1-1B	24	24	0	0
D1-2A	30	36	-6	36
D1-2B	32	31.5	0.5	0.25
D2-1A	16	29	-13	169
D2-1B	25	28	-3	9
EC-1A	27	27	0	0
EC-1B	29	26	3	9
EC-2A	19	15	4	16
EC-2B	36	23	13	169
EC-3A	22	11	11	121
EC-3B	8	12	-4	16
EC-4A	10	9	1	1
EC-4B	20	18	2	4
LC-1A	31	41	-10	100
LC-1B	13	40	-27	729
MC-1A	17	17	0	0
MC-1B	18	30	-12	144
MC-2A	26	25	1	1
MC-2B	23	14	9	81
MC-3A	35	22	13	169
MC-3B	33	15	20	400
PC-1A	7	8	-1	1
PC-1B	12	10	2	4
PC-2A	37	37	0	0
PC-2B	38	39	-1	1
PC-3A	44	34	10	100
PC-3B	45	42	3	9

$$r_s = 1 - \frac{6\sum d_i^2}{n(n^2-1)}$$

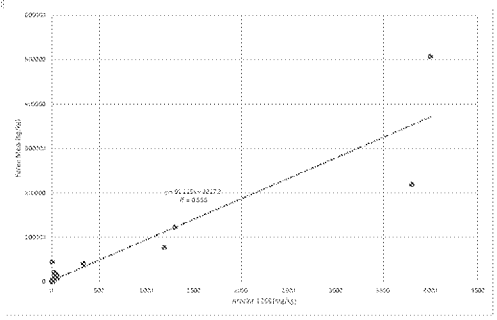
n=	46
r_s=	0.706





Case 2b: Co-location of Furan Congener Concentration and Aroclor 1268 (Cumulative Data Set)

Location	X: Ar1268 (mg/kg)	Y: Furans (ng/kg)
56	55	14468
61	1500	122400
68	330	40850
1718	56	8750
BR048	1.4	591
C-15	0.10	1548
C-5	8	44710
C-8	2	2826
111	6	5036
EPA-E3	3800	219000
EPA-F2	1188	77700
EPA-H1	8000	507600
GRID MARSH	6	3690
117	11.0	148
110	0.25	630
100	1.1	71
101	0.09	161
102	0.13	147
D1-1A	2.3	1206
D1-1B	5.1	1641
D1-2A	1.4	565
D1-2B	2.3	600
D2-1A	5.0	5831
D2-1B	5	5162
EC-1A	4.5	999
EC-1B	4.6	1002
EC-2A	12.6	2030
EC-2B	5.7	230
EC-3A	24.4	3810
EC-3B	22	20737
EC-4A	29	17069
EC-4B	6	3446
LC-1A	1	728
LC-1B	1.0	2958
MC-1A	9	2088
MC-1B	2.9	1409
MC-2A	5.0	1515
MC-2B	14.2	2089
MC-3A	5.7	1356
MC-3B	18.0	1872
PC-1A	51.1	15310
PC-1B	25	4611
PC-2A	1	649
PC-2B	1.0	207
PC-3A	1.9	316
PC-3B	0.6	206



Regression Analysis
SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.911664686
R Square	0.867999086
Adjusted R Square	0.864999067
Standard Error	50164.6145
Observations	46

H_0 = Furan mass not correlated to Aroclor 1268
H_a = Furan mass correlated to Aroclor 1268
p=0.05
Status: Furan mass correlated to Aroclor 1268

ANOVA

	df	SS	MS	F	Significance F
Regression	1	2.63263E+11	2.63263E+11	289.3810295	5.75115E-21
Residual	44	40035774057	909903956.1		
Total	45	3.05299E+11			

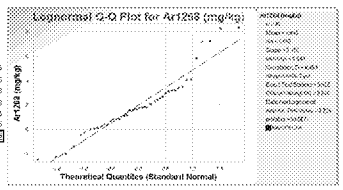
	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	2817.328485	4632.550728	0.608159232	0.546208528	-6518.96405	12155.62162	-6518.96405	12155.62162
Ar1268 (mg/kg)	92.11593293	5.415448573	17.00973838	5.75115E-21	81.20121588	103.029452	81.20121588	103.029452

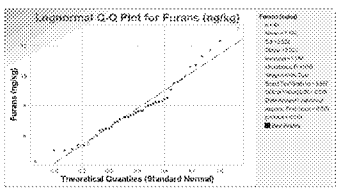
Pearson Correlation Analysis

Location	Log X	Log Y	(Log X)²	(Log Y)²	LOG X * LOG Y
56	1.7	4.2	3.028862291	17.30899887	7.240619722
61	3.1	5.1	9.696545201	25.88551971	15.84506311
68	2.5	4.6	6.542912465	21.26509213	11.61355145
1718	1.7	3.9	3.056151378	15.5394275	6.691371284
BR048	0.1	2.6	0.021355403	6.71938035	0.378789698
C-15	-1.0	3.1	1.008748662	9.794958832	-3.143350381
C-5	0.9	4.7	0.773817911	21.62626356	4.09081777 8
C-8	0.3	3.5	0.117253292	11.91053934	1.181759611
111	0.8	3.7	0.61574295	13.70541041	2.907383655
EPA-E3	3.6	5.3	12.8148506	28.52457778	19.11905339
EPA-F2	3.1	4.9	9.454495144	23.91621774	15.05714695
EPA-H1	3.6	5.7	12.97489618	32.59297688	20.55163113
GRID MARSH	0.8	3.6	0.61574295	12.72967703	2.801292221
117	1.0	2.2	1.084498725	4.70503774	2.258895179
110	-0.6	2.8	0.362476233	7.836907512	-1.685370947
100	0.0	1.8	0.001713354	3.415803012	-0.07650151
101	-1.1	2.2	1.146143837	4.871258925	-2.362871829
102	-0.9	2.2	0.785093683	4.701767894	-1.921285279
D1-1A	0.4	3.1	0.129481574	9.494701251	1.108778095
D1-1B	0.7	3.2	0.503055878	10.33692319	2.280579958
D1-2A	0.1	2.8	0.018592515	7.571654475	0.376209055
D1-2B	0.4	2.8	0.129481574	7.719732652	0.999781544
D2-1A	0.5	3.5	0.251787005	12.84012598	1.725159221
D2-1B	0.5	3.5	0.257817586	12.24973506	1.777476184
EC-1A	0.7	3.0	0.425425289	8.997914573	1.995512319
EC-1B	0.7	3.0	0.43674318	9.004426587	1.983083937
EC-2A	1.1	3.3	1.210613037	10.95953004	3.639471218
EC-2B	0.8	2.4	0.567887427	5.576863313	1.779615762
EC-3A	1.4	3.6	1.92485053	12.82902568	4.95813868
EC-3B	1.3	4.3	1.807930586	18.6342954	5.605399873
EC-4A	1.5	4.2	2.129826433	17.91072367	6.176904131
EC-4B	0.9	3.5	0.781890517	12.51259934	3.127795932
LC-1A	-0.1	2.9	0.020182389	8.192478924	-0.406624684
LC-1B	0.0	3.5	0.000253541	12.04782829	-0.055268586
MC-1A	1.0	3.3	0.942475184	11.02199125	3.223054785
MC-1B	0.5	3.1	0.208259956	9.915604443	1.457050019
MC-2A	0.7	3.2	0.486128756	10.11562452	2.21747701
MC-2B	1.2	3.3	1.327768429	11.02199125	3.825526358
MC-3A	0.8	3.1	0.569041412	9.815050969	2.363297727
MC-3B	1.3	3.3	1.757509062	10.70795554	4.107835555
PC-1A	1.5	4.1	2.238333579	17.00884463	6.156409630
PC-1B	1.4	3.7	1.92378241	13.4235947	5.089619924
PC-2A	0.1	2.8	0.008727611	7.909849144	0.262743389
PC-2B	0.0	2.3	0.000154794	5.560801523	0.029722546
PC-3A	0.3	2.5	0.076451129	6.249809329	0.691143598
PC-3B	-0.2	2.3	0.047944822	5.355932006	-0.506748575

$$r = \frac{n(\sum xy) - (\sum x)(\sum y)}{\sqrt{[n(\sum x^2) - (\sum x)^2][n(\sum y^2) - (\sum y)^2]}}$$

$\sum$LOG X	98.80771185
$\sum$(LOG X)^2	83.87978646
$\sum$LOG Y	155.7068408
$\sum$(LOG Y)^2	561.7602278
$\sum$(LOG X x Log Y)	167.0159133
n	46
r	0.846





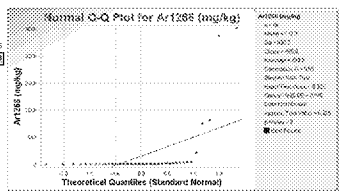
Pearson Correlation not applicable- variables do not follow normal/lognormal distribution

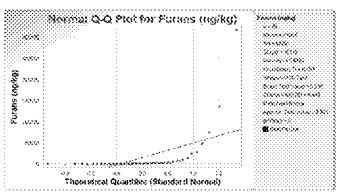
Spearman Correlation Analysis

Location	Ar1268 Rank	Furans Rank	Rank Difference	Difference^2
56	7	9	-2	4
61	5	5	0	0
68	5	6	-1	1
1718	6	11	-5	25
BR048	55	38	-5	9
C-15	45	29	16	256
C-5	19	5	14	196
C-8	33	20	13	169
111	20.5	12	8.5	72.25
EPA-E3	2	2	0	0
EPA-F2	4	4	0	0
EPA-H1	1	1	0	0
GRID MARSH	20.5	16	4.5	20.25
117	16	44	-28	784
110	43	35	8	64
100	38	46	-8	64
101	46	43	3	9
102	44	45	-1	1
D1-1A	31.5	30	1.5	2.25
D1-1B	24	25	-1	1
D1-2A	36	37	-1	1
D1-2B	31.5	36	-4.5	20.25
D2-1A	29	14	15	225
D2-1B	28	18	10	100
EC-1A	27	32	-5	25
EC-1B	26	31	-5	25
EC-2A	15	23	-8	64
EC-2B	23	40	-17	289
EC-3A	11	15	-4	16
EC-3B	12	7	5	25
EC-4A	9	8	1	1
EC-4B	18	17	1	1
LC-1A	41	33	8	64
LC-1B	40	19	21	441
MC-1A	17	21.5	-4.5	20.25
MC-1B	30	27	3	9
MC-2A	25	26	-1	1
MC-2B	14	21.5	-7.5	56.25
MC-3A	22	28	-6	36
MC-3B	13	24	-11	121
PC-1A	8	10	-2	4
PC-1B	10	13	-3	9
PC-2A	37	34	3	9
PC-2B	39	41	-2	4
PC-3A	34	39	-5	25
PC-3B	42	42	0	0

$$r_s = 1 - \frac{6\sum d_i^2}{n(n^2-1)}$$

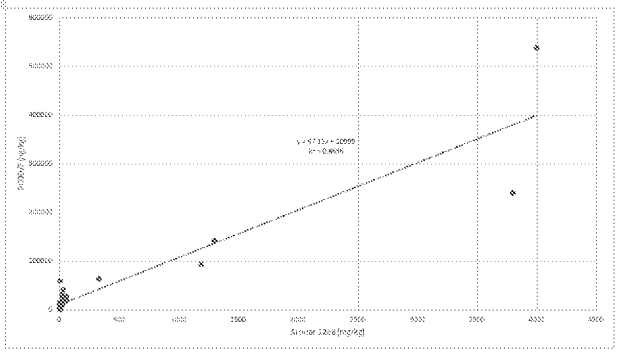
n=	46
r_s=	0.798





Case 3a: Co-location of PCDD/F Concentration and Aroclor 1268 (Original Distribution)

Location	Y- PCDD/F (pg/kg)	X- Ar1268 (mg/kg)
36	27038	55
61	141906	1300
68	64192	330
1716	18409	56
BR046	2981	1.4
C-15	10634	0.099
C-6	59189	7.58
111	9396	6.1
EPA-E3	240328	3800
EPA-F2	94068	1188
EPA-H1	536204	4000
GRID MARSH	5960	6.1
117	2133	11
110	3049	0.25
100	856	1.1
101	2058	0.085
102	2678	0.13
D2-1A	10471	3.03
D2-1B	8782	3.22
EC-3A	9244	24.4
EC-3B	31228	22.1
EC-4A	26257	28.8
EC-4B	9796	7.66
LC-1A	6639	0.721
LC-1B	15394	0.964
PC-1A	40766	31.1
PC-1B	18361	24.5
PC-2A	3534	1.24
PC-2B	3473	1.03
PC-3A	1691	1.69
PC-3B	1128	0.604
D1-2A	6945	1.37
D1-2B	6285	2.29



Regression Analysis
SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.929288027
R Square	0.863578236
Adjusted R Square	0.85917547
Standard Error	38015.98318
Observations	33

H_0 = PCDD/F not correlated to Aroclor 1268
H_A = PCDD/F correlated to Aroclor 1268
$p<0.05$
Status: PCDD/F correlated to Aroclor 1268

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	2.83599E+11	2.83599E+11	196.2331389	5.93396E-15
Residual	31	44801664291	1445214977		
Total	32	3.28401E+11			

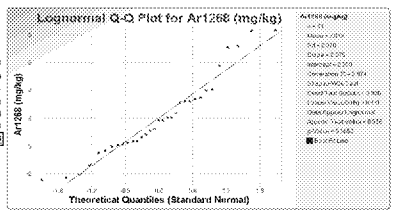
	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	10998.59331	7004.20235	1.570284918	0.126501041	-3286.571562	25283.75818	-3286.571562	25283.75818
Ar1268 (mg/kg)	97.15010107	6.935169523	14.00832391	5.93396E-15	83.00572958	111.2944726	83.00572958	111.2944726

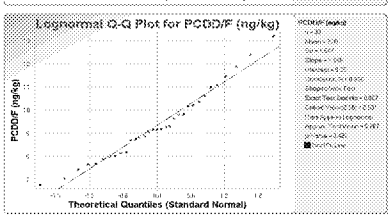
Pearson Correlation Analysis

Location	Log X	Log Y	$(\text{Log X})^2$	$(\text{Log Y})^2$	LOG X * LOG Y
36	1.7	4.4	3.028862291	19.64238427	7.713240372
61	3.1	5.2	9.696643201	26.54311177	16.0430385
68	2.5	4.8	6.342912465	23.11187261	12.10770766
1716	1.7	4.2	3.056181378	18.19052286	7.45608298
BR046	0.1	3.5	0.021353403	12.07119115	0.507701691
C-15	-1.0	4.0	1.006746862	16.2795209	-4.052399698
C-6	0.9	4.8	0.773817911	22.77428413	4.157993446
111	0.8	4.0	0.61674295	15.76441093	3.120083998
EPA-E3	3.6	5.4	12.8148506	28.95305958	19.26211052
EPA-F2	3.1	5.0	9.454496144	24.73602903	15.29270058
EPA-H1	3.6	5.7	12.97483618	32.84375446	20.6432152
GRID MARSH	0.8	3.8	0.61674295	14.26347177	2.965956111
117	1.0	3.3	1.064496725	11.08274061	3.466874394
110	-0.6	3.5	0.362476233	12.13895591	-2.097637484
100	0.0	2.9	0.001713354	8.598509567	0.12137666
101	-1.1	3.3	1.146143837	10.9763524	-3.547220171
102	-0.9	3.4	0.785096363	11.74990422	-3.037236768
D2-1A	0.5	4.0	0.231787005	16.16017141	1.935365679
D2-1B	0.5	3.9	0.257917586	15.55196817	2.002779592
EC-3A	1.4	4.0	1.92485053	15.76502022	5.508657508
EC-3B	1.3	4.5	1.807390586	20.20097731	6.042437935
EC-4A	1.5	4.4	2.129826433	19.52975653	6.449417934
EC-4B	0.9	4.0	0.781660517	15.92928417	3.529090301
LC-1A	-0.1	3.8	0.020182389	14.70702215	-0.544614503
LC-1B	0.0	4.2	0.000253541	17.53386518	-0.066674966
PC-1A	1.5	4.6	2.228333579	21.25487804	6.882075156
PC-1B	1.4	4.3	1.92976241	18.18077158	5.923253598
PC-2A	0.1	3.5	0.008727611	12.5905443	0.331485632
PC-2B	0.0	3.5	0.000164794	12.53685601	0.045453304
PC-3A	0.3	3.2	0.076431129	10.42091115	0.892458406
PC-3B	-0.2	3.1	0.047944822	9.315580021	-0.668306687
D1-2A	0.1	3.8	0.018692513	14.75839763	0.525234754
D1-2B	0.4	3.8	0.129481574	14.42733298	1.366774959

$$r = \frac{n(\sum xy) - (\sum x)(\sum y)}{\sqrt{[n(\sum x^2) - (\sum x)^2][n(\sum y^2) - (\sum y)^2]}}$$

$\sum$LOG X	28.94280213
$\sum(\text{LOG X})^2$	75.37972369
$\sum$LOG Y	134
$\sum(\text{LOG Y})^2$	558.605413
$\sum$(LOG X x Log Y)	140.3183064
n	33
r	**0.848**



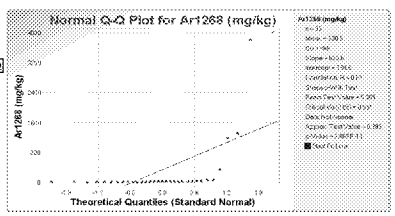


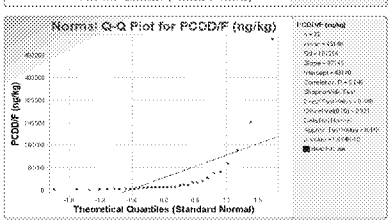
Spearman Correlation Analysis

Location	PCDD/F Rank	Ar1268 Rank	Rank Difference	Difference^2
36	9	7	2	4
61	3	3	0	0
68	5	5	0	0
1716	11	6	5	25
BR046	27	22	5	25
C-15	14	32	-18	324
C-6	6	15	-9	81
111	17	16.5	0.5	0.25
EPA-E3	2	2	0	0
EPA-F2	4	4	0	0
EPA-H1	1	1	0	0
GRID MARSH	23	16.5	6.5	42.25
117	29	13	16	256
110	26	30	-4	16
100	33	25	8	64
101	30	33	-3	9
102	28	31	-3	9
D2-1A	15	19	-4	16
D2-1B	19	18	1	1
EC-3A	18	11	7	49
EC-3B	8	12	-4	16
EC-4A	10	9	1	1
EC-4B	16	14	2	4
LC-1A	21	28	-7	49
LC-1B	13	27	-14	196
PC-1A	7	8	-1	1
PC-1B	12	10	2	4
PC-2A	24	24	0	0
PC-2B	25	26	-1	1
PC-3A	31	21	10	100
PC-3B	32	29	3	9
D1-2A	20	23	-3	9
D1-2B	22	20	2	4

$$r_s = 1 - \frac{6\sum d_i^2}{n(n^2-1)}$$

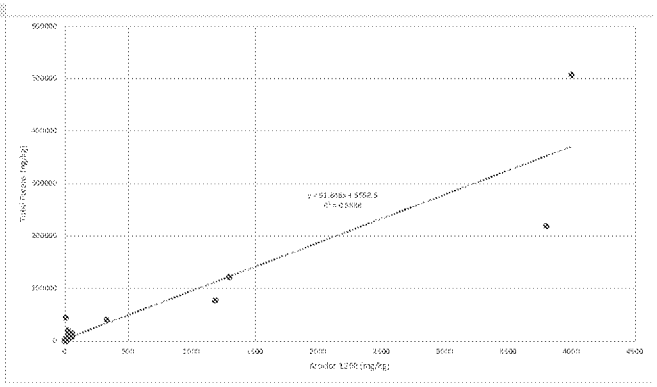
n=	33
r_s=	**0.780**





Case 3b: Co-location of Furan Mass and Aroclor 1268 (Original Distribution)

Location	X- Ar1268 (mg/kg)	Y- Furans (ng/kg)
36	55	14468
61	1300	122400
68	330	40850
1718	56	8750
BR048	1.4	391
C-15	0.1	1348
C-6	8	44710
111	6	5036
EPA-E3	3800	219200
EPA-F2	1188	77700
EPA-H1	4000	507600
GRID MARSH	6	3690
117	11.0	148
110	0.25	630
100	1.1	71
101	0.1	161
102	0.1	147
D2-1A	3.0	3831
D2-1B	3	3162
EC-3A	24.4	3810
EC-3B	22	20737
EC-4A	29	17065
EC-4B	8	3446
LC-1A	1	728
LC-1B	1.0	2958
PC-1A	31.1	13310
PC-1B	25	4611
PC-2A	1	649
PC-2B	1.0	207
PC-3A	1.9	316
PC-3B	0.6	206
D1-2A	1.37	565
D1-2B	2.29	600



Regression Analysis
SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.929419365
R Square	0.863820356
Adjusted R Square	0.859427465
Standard Error	35904.05431
Observations	33

H_0 = Furan mass not correlated to Aroclor 1268
H_A = Furan mass correlated to Aroclor 1268
$p<0.05$
Status: Furan mass correlated to Aroclor 1268

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	2.53489E+11	2.53489E+11	196.6404842	5.77075E-15
Residual	31	39962134596	1289101116		
Total	32	2.93452E+11			

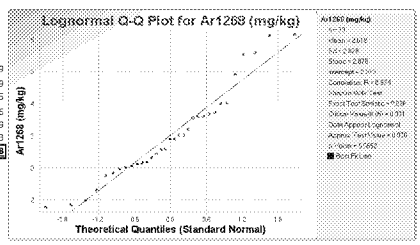
	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	3658.299321	6615.09293	0.553023118	0.58421401	-9833.27166	17149.8703	-9833.27166	17149.8703
Ar1268 (mg/kg)	91.84823482	6.549895133	14.02285578	5.77075E-15	78.48963563	105.206834	78.48963563	105.206834

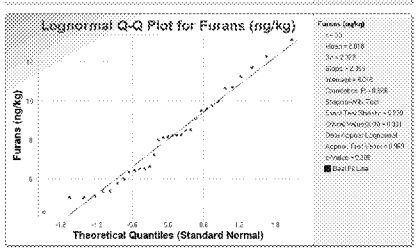
Pearson Correlation Analysis

Location	Log X	Log Y	$(\text{Log X})^2$	$(\text{Log Y})^2$	LOG X * LOG Y
36	1.7	4.2	3.028862291	17.30899887	7.240619722
61	3.1	5.1	9.696643201	25.88551971	15.84306311
68	2.5	4.6	6.342912465	21.26309213	11.61335146
1718	1.7	3.9	3.056161378	15.5394275	6.891371284
BR048	0.1	2.6	0.021353403	6.71938035	0.378789658
C-15	-1.0	3.1	1.008748662	9.794958832	-3.143350381
C-6	0.9	4.7	0.773817911	21.62626356	4.090817778
111	0.8	3.7	0.61674295	13.70549041	2.907363855
EPA-E3	3.6	5.3	12.8148506	28.52457778	19.11905339
EPA-F2	3.1	4.9	9.454496144	23.91621774	15.03714695
EPA-H1	3.6	5.7	12.97483618	32.55297688	20.55163113
GRID MARSH	0.8	3.6	0.61674295	12.72367703	2.801292221
117	1.0	2.2	1.084498725	4.70503774	2.258895179
110	-0.6	2.8	0.362476233	7.836307512	-1.685370947
100	0.0	1.8	0.001713354	3.415803012	0.07650151
101	-1.1	2.2	1.146143837	4.871258825	-2.362871829
102	-0.9	2.2	0.785096383	4.701767894	-1.921286279
D2-1A	0.5	3.6	0.231787005	12.84012598	1.725159221
D2-1B	0.5	3.5	0.257917586	12.24973306	1.777476184
EC-3A	1.4	3.6	1.92485053	12.82302368	4.96813888
EC-3B	1.3	4.3	1.807390586	18.6342954	5.803399873
EC-4A	1.5	4.2	2.129826433	17.91072367	6.176304131
EC-4B	0.9	3.5	0.781860517	12.51259934	3.127795932
LC-1A	-0.1	2.9	0.020182389	8.192478924	-0.406624884
LC-1B	0.0	3.5	0.000253541	12.04782829	-0.055268586
PC-1A	1.5	4.1	2.228333579	17.00884463	6.156409639
PC-1B	1.4	3.7	1.92978241	13.4233947	5.089619924
PC-2A	0.1	2.8	0.008727611	7.909840144	0.262743389
PC-2B	0.0	2.3	0.000164794	5.360801523	0.029722546
PC-3A	0.3	2.5	0.076431129	6.249809329	0.691143968
PC-3B	-0.2	2.3	0.047944822	5.355932006	0.50674373
D1-2A	0.1	2.8	0.018692513	7.571654473	0.376209055
D1-2B	0.4	2.8	0.129481574	7.719732632	0.999781544

$$r = \frac{n(\sum xy) - (\sum x)(\sum y)}{\sqrt{[n(\sum x^2) - (\sum x)^2][n(\sum y^2) - (\sum y)^2]}}$$

∑LOG X	29
$\sum(\text{LOG X})^2$	75.37972369
∑LOG Y	115
$\sum(\text{LOG Y})^2$	432.9015826
∑(LOG X x Log Y)	135.9122849
n	33
r	**0.868**



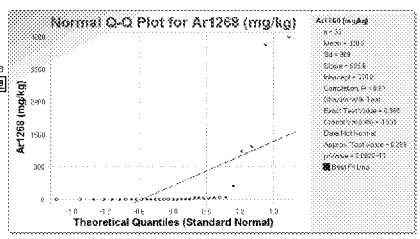


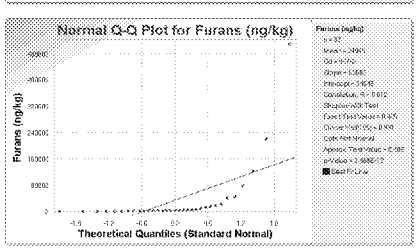
Spearman Correlation Analysis

Location	Aroclor 1268 Rank	Furans Rank	Rank Difference	Difference^2
36	7	9	-2	4
61	3	3	0	0
68	5	6	-1	1
1718	6	11	-5	25
BR048	22	26	-4	16
C-15	32	20	12	144
C-6	15	5	10	100
111	16.5	12	4.5	20.25
EPA-E3	2	2	0	0
EPA-F2	4	4	0	0
EPA-H1	1	1	0	0
GRID MARSH	16.5	16	0.5	0.25
117	13	31	-18	324
110	30	23	7	49
100	25	33	-8	64
101	33	30	3	9
102	31	32	-1	1
D2-1A	19	14	5	25
D2-1B	18	18	0	0
EC-3A	11	15	-4	16
EC-3B	12	7	5	25
EC-4A	9	8	1	1
EC-4B	14	17	-3	9
LC-1A	28	21	7	49
LC-1B	27	19	8	64
PC-1A	8	10	-2	4
PC-1B	10	13	-3	9
PC-2A	24	22	2	4
PC-2B	26	28	-2	4
PC-3A	21	27	-6	36
PC-3B	29	29	0	0
D1-2A	23	25	-2	4
D1-2B	20	24	-4	16

$$r_s = 1 - \frac{6\sum d_i^2}{n(n^2-1)}$$

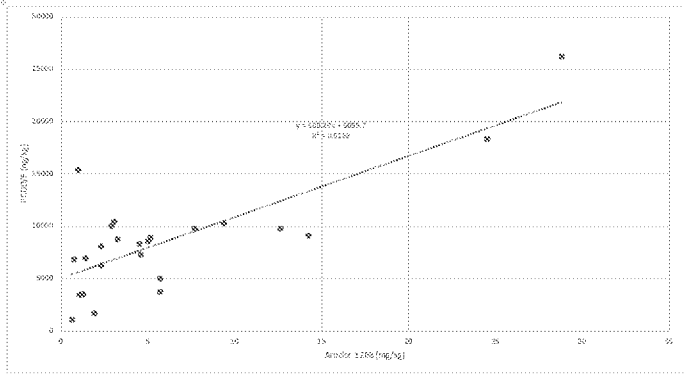
n=	33
r_s=	**0.829**





Case 1a: Co-location of PCDD/F Concentration and Aroclor 1268, Excluding Outliers (Co-location Study Data)

Location	Y- PCDD/F (ng/kg)	X- Ar1268 (mg/kg)
D1-1A	8114.0	2.29
D1-1B	8943.5	5.12
D1-2A	6944.9	1.37
D1-2B	6285.4	2.29
D2-1A	10470.6	3.03
D2-1B	8782.1	3.22
EC-1A	8337.3	4.49
EC-1B	7319.9	4.58
EC-2A	9803.0	12.6
EC-2B	3760.2	5.67
EC-4A	26257.2	28.8
EC-4B	9798.3	7.66
LC-1A	6838.7	0.721
LC-1B	15393.8	0.964
MC-1A	10308.4	9.35
MC-1B	10040.3	2.86
MC-2A	8594.3	4.98
MC-2B	9115.8	14.2
MC-3A	5032.9	5.68
PC-1B	18360.8	24.5
PC-2A	3534.4	1.24
PC-2B	3473.3	1.03
PC-3A	1691.0	1.89
PC-3B	1127.6	0.604



Regression Analysis

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.785379379
R Square	0.616820769
Adjusted R Square	0.599403531
Standard Error	3415.177045
Observations	24

H_0 = PCDD/F not correlated to Aroclor 1268
H_A = PCDD/F correlated to Aroclor 1268
$p<0.05$
Status: PCDD/F correlated to Aroclor 1268

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	413053353.4	413053353.4	35.41438521	5.46379E-06
Residual	22	256595553.5	11663434.25		
Total	23	669648906.9			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	5055.696672	925.7173154	5.461382852	1.73705E-05	3135.876463	6975.516881	3135.876463	6975.516881
Ar1268 (mg/kg)	583.2877374	98.01510124	5.950998673	5.46379E-06	380.0168587	786.5586162	380.0168587	786.5586162

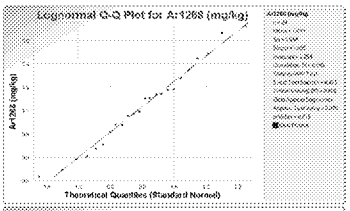
Pearson Correlation Analysis

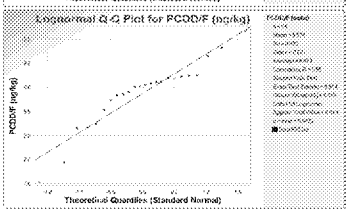
Location	Log X	Log Y	$(\text{Log X})^2$	$(\text{Log Y})^2$	LOG X * LOG Y
D1-1A	0.4	3.9	0.129481574	15.28211831	1.406681463
D1-1B	0.7	4.0	0.503063878	15.61441161	2.802685578
D1-2A	0.1	3.8	0.018692513	14.75839763	0.525234754
D1-2B	0.4	3.8	0.129481574	14.42733298	1.366774959
D2-1A	0.5	4.0	0.231787005	16.16017141	1.935385679
D2-1B	0.5	3.9	0.257917586	15.55196817	2.002779592
EC-1A	0.7	3.9	0.425425289	15.37444041	2.557474489
EC-1B	0.7	3.9	0.43674318	14.93440004	2.553918042
EC-2A	1.1	4.0	1.210815337	15.93094669	4.391973881
EC-2B	0.8	3.6	0.567887427	12.7821333	2.6942184
EC-4A	1.5	4.4	2.129826433	19.52975653	6.449417934
EC-4B	0.9	4.0	0.781860517	15.92928417	3.529090301
LC-1A	-0.1	3.8	0.020182389	14.70702215	-0.544814503
LC-1B	0.0	4.2	0.000253541	17.53386518	-0.066674966
MC-1A	1.0	4.0	0.942475184	16.10570411	3.896052674
MC-1B	0.5	4.0	0.208269956	16.01397657	1.826261262
MC-2A	0.7	3.9	0.486128756	15.47801233	2.743047008
MC-2B	1.2	4.0	1.327768429	15.67997476	4.562825381
MC-3A	0.8	3.7	0.569041412	13.70345874	2.792460475
PC-1B	1.4	4.3	1.92978241	18.18077158	5.923253598
PC-2A	0.1	3.5	0.008727611	12.5905443	0.331489632
PC-2B	0.0	3.5	0.000164794	12.53685601	0.045453304
PC-3A	0.3	3.2	0.076431129	10.42091115	0.892458406
PC-3B	-0.2	3.1	0.047944822	9.315580021	-0.668306687

Pearson Correlation not applicable- variables not normally/lognormally distributed

$$r = \frac{n\sum xy - \sum(x)\sum(y)}{\sqrt{\left[n\sum x^2 - (\sum x)^2\right]\left[n\sum y^2 - (\sum y)^2\right]}}$$

∑LOG X	13.49162638
$\sum(\text{LOG X})^2$	12.44015275
∑LOG Y	92.49312871
$\sum(\text{LOG Y})^2$	358.5420381
∑(LOG X x Log Y)	53.94914066
n	24
r_p	0.614



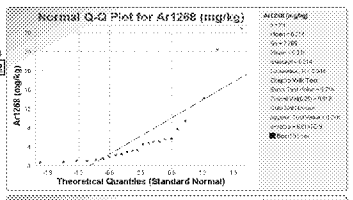


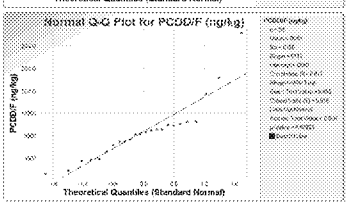
Spearman Correlation Analysis

Location	Furan Rank	Ar1268 Rank	Rank Difference	Difference^2
D1-1A	14	16.5	-2.5	6.25
D1-1B	10	9	1	1
D1-2A	16	19	-3	9
D1-2B	18	16.5	1.5	2.25
D2-1A	4	14	-10	100
D2-1B	11	13	-2	4
EC-1A	13	12	1	1
EC-1B	15	11	4	16
EC-2A	7	4	3	9
EC-2B	20	8	12	144
EC-4A	1	1	0	0
EC-4B	8	6	2	4
LC-1A	17	23	-6	36
LC-1B	3	22	-19	361
MC-1A	5	5	0	0
MC-1B	6	15	-9	81
MC-2A	12	10	2	4
MC-2B	9	3	6	36
MC-3A	19	7	12	144
PC-1B	2	2	0	0
PC-2A	21	20	1	1
PC-2B	22	21	1	1
PC-3A	23	18	5	25
PC-3B	24	24	0	0

$$r_s = 1 - \frac{6\sum d_i^2}{n(n^2-1)}$$

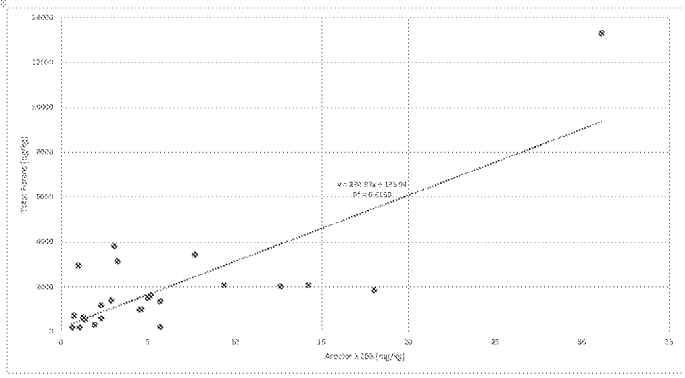
n=	24
r_s=	0.572





Case 1b: Co-location of Furan Congener Concentration and Aroclor 1268, Excluding Outliers (Co-location Study Data)

Location	Y- Furans (ng/kg)	X- Ar1268 (mg/kg)
D1-1A	1206.0	2.29
D1-1B	1641.0	5.12
D1-2A	564.5	1.37
D1-2B	600.4	2.29
D2-1A	3831.0	3.03
D2-1B	3162.0	3.22
EC-1A	999.2	4.49
EC-1B	1001.7	4.58
EC-2A	2030.0	12.6
EC-2B	229.9	5.67
EC-4B	3446.0	7.66
LC-1A	728.2	0.721
LC-1B	2958.0	0.964
MC-1A	2089.0	9.35
MC-1B	1409.0	2.86
MC-2A	1515.0	4.98
MC-2B	2089.0	14.2
MC-3A	1358.0	5.68
MC-3B	1872.0	18
PC-1A	13310.0	31.1
PC-2A	649.3	1.24
PC-2B	206.7	1.03
PC-3A	316.2	1.89
PC-3B	206.2	0.604



Regression Analysis

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.784394877
R Square	0.615275323
Adjusted R Square	0.597787838
Standard Error	1668.871447
Observations	24

H_0 = Furan mass not correlated to Aroclor 1268

H_a = Furan mass correlated to Aroclor 1268

$p<0.05$

Status: Furan mass correlated to Aroclor 1268

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	97991386.55	97991386.55	35.18375066	5.71744E-06
Residual	22	61272901.94	2785131.907		
Total	23	159264288.5			

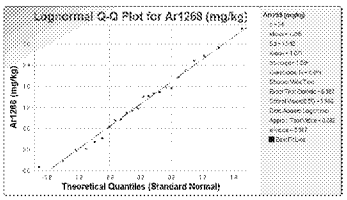
	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	195.0351234	454.0635536	0.429532654	0.671713165	-746.6350514	1136.705298	-746.6350514	1136.705298
Ar1268 (mg/kg)	294.8651297	49.71098282	5.931589219	5.71744E-06	191.7708613	397.9593982	191.7708613	397.9593982

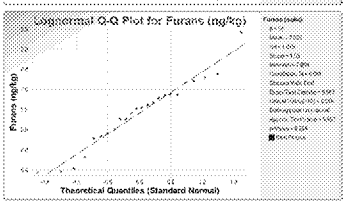
Pearson Correlation Analysis

Location	Log X	Log Y	$(\text{Log X})^2$	$(\text{Log Y})^2$	LOG X * LOG Y
D1-1A	0.4	3.1	0.1295	9.5	1.108778095
D1-1B	0.7	3.2	0.503063878	10.33692319	2.280379938
D1-2A	0.1	2.8	0.018692513	7.571654473	0.376209055
D1-2B	0.4	2.8	0.129481574	7.719732632	0.999781544
D2-1A	0.5	3.6	0.231787005	12.84012598	1.725159221
D2-1B	0.5	3.5	0.257917586	12.24973306	1.777476184
EC-1A	0.7	3.0	0.425425289	8.997914673	1.956512319
EC-1B	0.7	3.0	0.43674318	9.004426587	1.983083937
EC-2A	1.1	3.3	1.210815337	10.93953004	3.639471218
EC-2B	0.8	2.4	0.567887427	5.576866313	1.779615762
EC-4B	0.9	3.5	0.781860517	12.51259934	3.127795932
LC-1A	-0.1	2.9	0.020182389	8.192478924	-0.406624884
LC-1B	0.0	3.5	0.000253541	12.04782829	-0.055268586
MC-1A	1.0	3.3	0.942475184	11.02199125	3.223034785
MC-1B	0.5	3.1	0.208269956	9.915640443	1.437056019
MC-2A	0.7	3.2	0.486128756	10.11502452	2.21747701
MC-2B	1.2	3.3	1.327768429	11.02199125	3.825526368
MC-3A	0.8	3.1	0.569041412	9.815060969	2.363297727
MC-3B	1.3	3.3	1.575709062	10.70798554	4.107635555
PC-1A	1.5	4.1	2.228333579	17.00884463	6.156409639
PC-2A	0.1	2.8	0.008727611	7.909849144	0.262743389
PC-2B	0.0	2.3	0.000164794	5.360801523	0.029722546
PC-3A	0.3	2.5	0.076431129	6.249809329	0.691143968
PC-3B	-0.2	2.3	0.047944822	5.355932006	-0.50674373

$$r = \frac{n(\sum xy) - (\sum x)(\sum y)}{\sqrt{[n(\sum x^2) - (\sum x)^2][n(\sum y^2) - (\sum y)^2]}}$$

∑LOG X	13.4
$\sum(\text{LOG X})^2$	12.1846
∑LOG Y	73.9
$\sum(\text{LOG Y})^2$	231.9674453
∑(LOG X x Log Y)	44.09967301
n	24
r_s	**0.625**



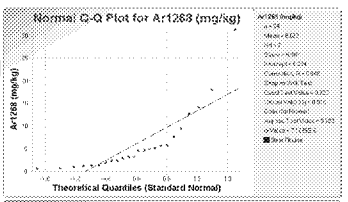


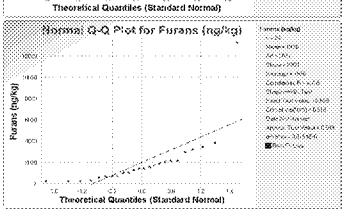
Spearman Correlation Analysis

Location	Furan Rank	Ar1268 Rank	Rank Difference	Difference^2
D1-1A	14	16.5	-2.5	6.25
D1-1B	10	9	1	1
D1-2A	20	19	1	1
D1-2B	19	16.5	2.5	6.25
D2-1A	2	14	-12	144
D2-1B	4	13	-9	81
EC-1A	16	12	4	16
EC-1B	15	11	4	16
EC-2A	8	4	4	16
EC-2B	22	8	14	196
EC-4B	3	6	-3	9
LC-1A	17	23	-6	36
LC-1B	5	22	-17	289
MC-1A	6.5	5	1.5	2.25
MC-1B	12	15	-3	9
MC-2A	11	10	1	1
MC-2B	6.5	3	3.5	12.25
MC-3A	13	7	6	36
MC-3B	9	2	7	49
PC-1A	1	1	0	0
PC-2A	18	20	-2	4
PC-2B	23	21	2	4
PC-3A	21	18	3	9
PC-3B	24	24	0	0

$$r_s = 1 - \frac{6\sum d_i^2}{n(n^2-1)}$$

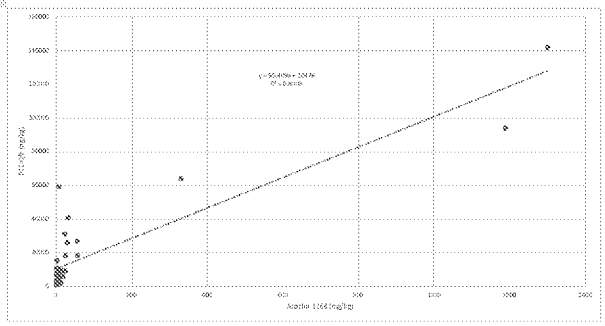
n=	24
r_s=	**0.590**





Case 2a: Co-location of PCDD/F Concentration and Aroclor 1268, Excluding Outliers (Cumulative Data Set)

Location	Y: PCDD/F (ng/kg)	X: Ar1268 (mg/kg)
36	27038	55
61	141906	1300
68	64192	330
1718	18409	56
BR048	2981	1.4
C-15	10834	0.099
C-6	59189	7.58
C-8	10654	2.2
111	9386	6.1
EPA-F2	94088	1188
GRID MARSH	5980	6.1
117	2133	11
110	3049	0.25
100	856	1.1
101	2058	0.085
102	2678	0.13
D1-1A	8114	2.29
D1-1B	8944	5.12
D1-2A	6945	1.37
D1-2B	6285	2.29
D2-1A	10471	3.03
D2-1B	8782	3.22
EC-1A	8337	4.49
EC-1B	7320	4.58
EC-2A	9803	12.6
EC-2B	3760	5.67
EC-3A	9344	24.4
EC-3B	31228	22.1
EC-4A	26257	28.8
EC-4B	9798	7.66
LC-1A	6839	0.721
LC-1B	15394	0.964
MC-1A	10308	9.35
MC-1B	10640	2.86
MC-2A	8594	4.98
MC-2B	9116	14.2
MC-3A	5033	5.68
MC-3B	6018	18
PC-1A	40766	31.1
PC-1B	18361	24.5
PC-2A	3534	1.24
PC-2B	3473	1.03
PC-3A	1691	1.89
PC-3B	1128	0.604



Regression Analysis
SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.894861803
R Square	0.800777646
Adjusted R Square	0.796034257
Standard Error	12025.98676
Observations	44

H_0 = PCDD/F not correlated to Aroclor 1268
H_a = PCDD/F correlated to Aroclor 1268
p<0.05
Status: PCDD/F correlated to Aroclor 1268

ANOVA

	df	SS	MS	F	Significance F
Regression	1	24415442899	24415442899	168.8197156	2.62815E-16
Residual	42	6074223015	144624357.5		
Total	43	30489665914			

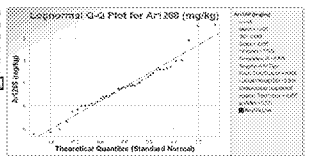
	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	10475.71343	1882.704909	5.564182355	1.67797E-06	6676.261105	14275.16576	6676.261105	14275.16576
X Variable 1	90.40918568	6.958265175	12.99306413	2.62815E-16	76.36683805	104.4515333	76.36683805	104.4515333

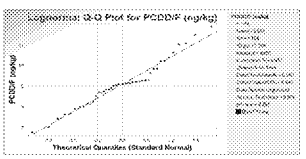
Pearson Correlation Analysis

Location	Log X	Log Y	$(\log X)^2$	$(\log Y)^2$	Log X * Log Y
36	1.7	4.4	3.028862291	19.64238427	7.713240372
61	3.1	5.2	9.696643201	26.54311177	16.0430385
68	2.5	4.8	6.342912465	23.11187261	12.10770766
1718	1.7	4.3	3.056181378	18.19052286	7.45608298
BR048	0.1	3.5	0.021353403	12.07119115	0.507701691
C-15	-1.0	4.0	1.008748662	16.2795209	-4.052399898
C-6	0.9	4.8	0.773817911	22.77428413	4.197993446
C-8	0.3	4.0	0.117253292	16.22098987	1.379117278
111	0.8	4.0	0.61674295	15.78441093	3.120083998
EPA-F2	3.1	5.0	9.454496144	24.73602903	15.29270058
GRID MARSH	0.8	3.8	0.61674295	14.26347177	2.965956111
117	1.0	3.3	1.084498725	11.08274061	3.466874394
110	-0.6	3.5	0.362476233	12.13895591	-2.097637484
100	0.0	2.9	0.001713354	8.598503567	0.121376662
101	-1.1	3.3	1.146143857	10.9783324	-3.547220171
102	-0.9	3.4	0.785096383	11.74990422	-3.037236788
D1-1A	0.4	3.9	0.129481574	15.28211831	1.406681463
D1-1B	0.7	4.0	0.503063878	15.61441161	2.802685578
D1-2A	0.1	3.8	0.018692513	14.75839763	0.525234754
D1-2B	0.4	3.8	0.129481574	14.42733298	1.366774959
D2-1A	0.5	4.0	0.231787005	16.16017141	1.935385679
D2-1B	0.5	3.9	0.257917586	15.55196817	2.002779592
EC-1A	0.7	3.9	0.425425289	15.37444041	2.557474489
EC-1B	0.7	3.9	0.43674318	14.93440004	2.553918042
EC-2A	1.1	4.0	1.210815337	15.93896069	4.391973881
EC-2B	0.8	3.6	0.567887427	12.7821333	2.6942184
EC-3A	1.4	4.0	1.92485053	15.76502022	5.508657508
EC-3B	1.3	4.5	1.807390586	20.20097731	6.042437935
EC-4A	1.5	4.4	2.129826433	19.52975653	6.449417934
EC-4B	0.9	4.0	0.781806517	15.92928417	3.529090301
LC-1A	-0.1	3.8	0.020182389	14.70702215	-0.544814503
LC-1B	0.0	4.2	0.000253541	17.53388518	-0.066674966
MC-1A	1.0	4.0	0.942475184	16.10570411	3.896052674
MC-1B	0.5	4.0	0.208269956	16.01397657	1.826261262
MC-2A	0.7	3.9	0.486128756	15.47801233	2.743047008
MC-2B	1.2	4.0	1.327768429	15.67997476	4.562825381
MC-3A	0.8	3.7	0.569041412	13.70345874	2.792460475
MC-3B	1.3	3.8	1.575709062	14.28442245	4.744269586
PC-1A	1.5	4.6	2.228333579	21.25487804	6.882075156
PC-1B	1.4	4.3	1.92978241	18.18077158	5.922535598
PC-2A	0.1	3.5	0.008727611	12.5905443	0.331489632
PC-2B	0.0	3.5	0.000164794	12.53685601	0.045453304
PC-3A	0.3	3.2	0.076431129	10.42091115	0.892458406
PC-3B	-0.2	3.1	0.047944822	9.315580021	-0.668306687

$$r = \frac{n(\sum xy) - (\sum x)(\sum y)}{\sqrt{[n(\sum x^2) - (\sum x)^2][n(\sum y^2) - (\sum y)^2]}}$$

$\sum$LOG X	31.62586826
$\sum$(LOG X)^2	58.09003968
$\sum$LOG Y	173.5232468
$\sum$(LOG Y)^2	694.2135882
$\sum$(LOG X x Log Y)	138.7639602
n	44
r	0.751



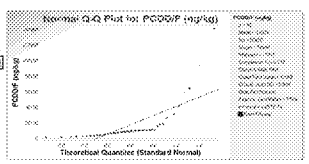


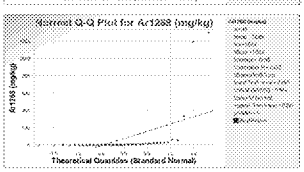
Spearman Correlation Analysis

Location	PCDD/F Rank	Ar1268 Rank	Rank Difference	D-Rifference^2
36	7	5	2	4
61	1	1	0	0
68	3	3	0	0
1718	9	4	5	25
BR048	38	33	5	25
C-15	12	43	-31	961
C-6	4	17	-13	169
C-8	13	31	-18	324
111	19	18.5	0.5	0.25
EPA-F2	2	2	0	0
GRID MARSH	32	18.5	13.5	182.25
117	40	14	26	676
110	37	41	-4	16
100	44	36	8	64
101	41	44	-3	9
102	39	42	-3	9
D1-1A	26	29.5	-3.5	12.25
D1-1B	22	22	0	0
D1-2A	28	34	-6	36
D1-2B	30	29.5	0.5	0.25
D2-1A	14	27	-13	169
D2-1B	23	26	-3	9
EC-1A	25	25	0	0
EC-1B	27	24	3	9
EC-2A	17	13	4	16
EC-2B	34	21	13	169
EC-3A	20	9	11	121
EC-3B	6	10	-4	16
EC-4A	8	7	1	1
EC-4B	18	16	2	4
LC-1A	29	39	-10	100
LC-1B	11	38	-27	729
MC-1A	15	15	0	0
MC-1B	16	28	-12	144
MC-2A	24	23	1	1
MC-2B	21	12	9	81
MC-3A	33	20	13	169
MC-3B	31	11	20	400
PC-1A	5	6	-1	1
PC-1B	10	8	2	4
PC-2A	35	35	0	0
PC-2B	36	37	-1	1
PC-3A	42	32	10	100
PC-3B	43	40	3	9

$$r_s = 1 - \frac{6\sum d^2}{n(n^2-1)}$$

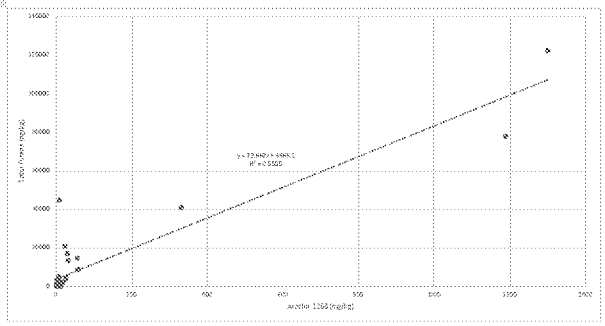
n=	44
r_s=	0.664





Case 2b: Co-location of Furan Congener Concentration and Aroclor 1268, Excluding Outliers (Cumulative Data Set)

Location	Y: Furans (mg/kg)	X: Ar1268 (mg/kg)
36	14468	55
61	122400	1300
68	40850	330
1718	8750	56
BR048	391	1.4
C-15	1348	0.1
C-6	44710	8
C-8	2826	2
111	5636	6
EPA-F2	77700	1188
GRID MARSH	3690	6
117	148	11.0
110	630	0.25
100	71	1.1
101	161	0.1
102	147	0.1
D1-1A	1206	2.3
D1-1B	1641	5.1
D1-2A	565	1.4
D1-2B	600	2.3
D2-1A	3831	3.0
D2-1B	3162	3
EC-1A	999	4.5
EC-1B	1002	4.6
EC-2A	2030	12.6
EC-2B	230	5.7
EC-3A	3810	24.4
EC-3B	20737	22
EC-4A	17655	29
EC-4B	3446	8
LC-1A	728	1
LC-1B	2958	1.0
MC-1A	2689	9
MC-1B	1469	2.9
MC-2A	1515	5.0
MC-2B	2089	14.2
MC-3A	1358	5.7
MC-3B	1872	18.0
PC-1A	13310	31.1
PC-1B	4611	25
PC-2A	649	1
PC-2B	267	1.0
PC-3A	316	1.9
PC-3B	206	0.6



Regression Analysis
SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.926537947
R Square	0.858472567
Adjusted R Square	0.855102866
Standard Error	8625.837656
Observations	44

H_0 = Furan mass not correlated to Aroclor 1268
H_a = Furan mass correlated to Aroclor 1268
p<0.05
Status: Furan mass correlated to Aroclor 1268

ANOVA

	df	SS	MS	F	Significance F
Regression	1	18955604694	18955604694	254.7622541	1.93601E-19
Residual	42	3125013162	74405075.27		
Total	43	22080617855			

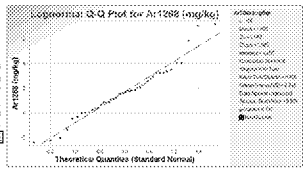
	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	3665.237682	1350.401196	2.714184268	0.009596386	940.0177371	6390.457627	940.0177371	6390.457627
X Variable 1	79.66160932	4.990930639	15.96127357	1.93601E-19	69.58950351	89.73371512	69.58950351	89.73371512

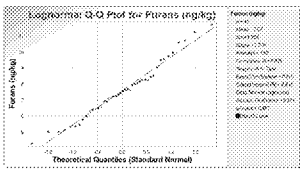
Pearson Correlation Analysis

Location	Log X	Log Y	$(\log X)^2$	$(\log Y)^2$	Log X * Log Y
36	1.7	4.2	3.028852291	17.30899887	7.240619722
61	3.1	5.1	9.696643201	25.88551971	15.84306311
68	2.5	4.6	6.342912465	21.26309213	11.61335146
1718	1.7	3.9	3.056181378	15.5394275	6.891371284
BR048	0.1	2.6	0.021353403	6.71938035	0.378789698
C-15	-1.0	3.1	1.008748662	9.794958832	-3.143350381
C-6	0.9	4.7	0.773817911	21.62626356	4.090817778
C-8	0.3	3.5	0.117253292	11.91058924	1.181759621
111	0.8	3.7	0.61674295	13.70549041	2.907363855
EPA-F2	3.1	4.9	9.454936144	23.91621774	15.03714695
GRID MARSH	0.8	3.6	0.61674295	12.72367703	2.801252221
117	1.0	2.2	1.084498725	4.70503774	2.258895179
110	-0.6	2.8	0.362476233	7.836307512	-1.685370947
100	0.0	1.8	0.001713354	3.415803012	0.07650151
101	-1.1	2.2	1.146143837	4.871258825	-2.362871829
102	-0.9	2.2	0.785096383	4.701767854	-1.921286279
D1-1A	0.4	3.1	0.129481574	9.494701231	1.108778095
D1-1B	0.7	3.2	0.503063878	10.33692319	2.280379938
D1-2A	0.1	2.8	0.018692513	7.571054473	0.376203055
D1-2B	0.4	2.8	0.129481574	7.719732632	0.998781544
D2-1A	0.5	3.6	0.231787005	12.84012598	1.725159221
D2-1B	0.5	3.5	0.257917586	12.24973306	1.777476184
EC-1A	0.7	3.0	0.425425289	8.997914673	1.956512319
EC-1B	0.7	3.0	0.43674318	9.004426587	1.983083937
EC-2A	1.1	3.3	1.210815337	10.93953004	3.639471218
EC-2B	0.8	2.4	0.567887427	5.576866313	1.779615762
EC-3A	1.4	3.6	1.92485053	12.82302368	4.96813888
EC-3B	1.3	4.3	1.807390586	18.6342954	5.803399873
EC-4A	1.5	4.2	2.129826433	17.91072367	6.176304131
EC-4B	0.9	3.5	0.781800517	12.51259934	3.127795932
LC-1A	-0.1	2.9	0.020182389	8.192478924	-0.406624884
LC-1B	0.0	3.5	0.000253541	12.04782829	-0.055268586
MC-1A	1.0	3.3	0.942475184	11.02199125	3.223034785
MC-1B	0.5	3.1	0.208269956	9.915640443	1.437056819
MC-2A	0.7	3.2	0.486128756	10.11502452	2.21747701
MC-2B	1.2	3.3	1.327768429	11.02199125	3.825526368
MC-3A	0.8	3.1	0.569041412	9.815060969	2.363297727
MC-3B	1.3	3.3	1.575709062	10.70798554	4.107635555
PC-1A	1.5	4.1	2.228333579	17.00884463	6.156403639
PC-1B	1.4	3.7	1.92978241	13.4233947	5.088619924
PC-2A	0.1	2.8	0.008727611	7.909849144	0.262743389
PC-2B	0.0	2.3	0.000164794	5.360801523	0.029722546
PC-3A	0.3	2.5	0.076431129	6.249809329	0.691143968
PC-3B	-0.2	2.3	0.047944822	5.355932006	-0.50674373

$$r = \frac{n\sum XY - (\sum X)(\sum Y)}{\sqrt{[n\sum X^2 - (\sum X)^2][n\sum Y^2 - (\sum Y)^2]}}$$

$\sum$Log X	31.62586826
$\sum(\text{LOG X})^2$	58.09009968
$\sum$LOG Y	144.6604787
$\sum(\text{LOG Y})^2$	506.6826731
$\sum$(LOG X x Log Y)	127.3452288
n	44
r	0.785



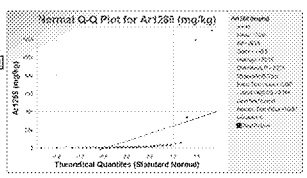


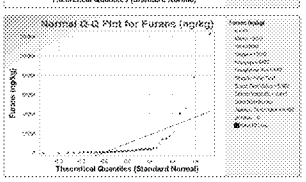
Spearman Correlation Analysis

Location	Ar1268 Rank	Furans Rank	Rank Difference	Difference^2
36	5	7	-2	4
61	1	1	0	0
68	3	4	-1	1
1718	4	9	-5	25
BR048	33	36	-3	9
C-15	43	27	16	256
C-6	17	3	14	196
C-8	31	18	13	169
111	18.5	10	8.5	72.25
EPA-F2	2	2	0	0
GRID MARSH	18.5	14	4.5	20.25
117	14	42	-28	784
110	41	33	8	64
100	36	44	-8	64
101	44	41	3	9
102	42	43	-1	1
D1-1A	29.5	28	1.5	2.25
D1-1B	22	23	-1	1
D1-2A	34	35	-1	1
D1-2B	29.5	34	-4.5	20.25
D2-1A	27	12	15	225
D2-1B	26	16	10	100
EC-1A	25	30	-5	25
EC-1B	24	29	-5	25
EC-2A	13	21	-8	64
EC-2B	21	38	-17	289
EC-3A	9	13	-4	16
EC-3B	10	5	5	25
EC-4A	7	6	1	1
EC-4B	16	15	1	1
LC-1A	39	31	8	64
LC-1B	38	17	21	441
MC-1A	15	19.5	-4.5	20.25
MC-1B	28	25	3	9
MC-2A	23	24	-1	1
MC-2B	12	19.5	-7.5	56.25
MC-3A	20	26	-6	36
MC-3B	11	22	-11	121
PC-1A	6	8	-2	4
PC-1B	8	11	-3	9
PC-2A	35	32	3	9
PC-2B	37	39	-2	4
PC-3A	32	37	-5	25
PC-3B	40	40	0	0

$$r_s = 1 - \frac{6\sum d_i^2}{n(n^2-1)}$$

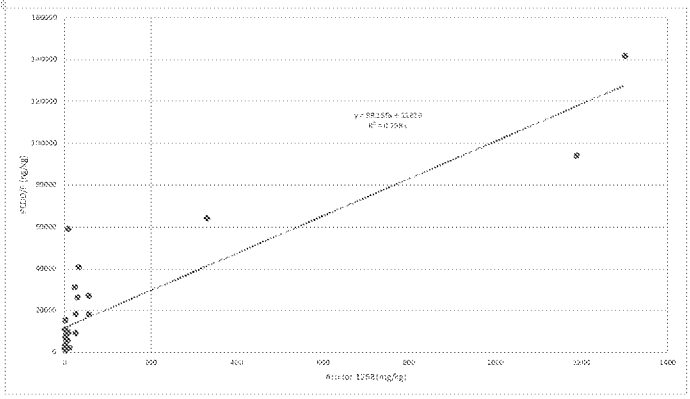
n=	44
r_s=	0.770





Case 3a: Co-location of PCDD/F Concentration and Aroclor 1268, Excluding Outliers (Original Distribution)

Location	Y- PCDD/F (ng/kg)	X- Ar1268 (mg/kg)
36	27038	55
61	141906	1300
68	64192	330
1718	18409	56
BR048	2981	1.4
C-15	10834	0.099
C-6	59189	7.58
111	9396	6.1
EPA-F2	94088	1188
GRID MARSH	5980	6.1
117	2133	11
110	3049	0.25
100	856	1.1
101	2058	0.085
102	2678	0.13
D2-1A	10471	3.03
D2-1B	8782	3.22
EC-3A	9344	24.4
EC-3B	31228	22.1
EC-4A	26257	28.8
EC-4B	9798	7.66
LC-1A	6839	0.721
LC-1B	15394	0.964
PC-1A	40766	31.1
PC-1B	18361	24.5
PC-2A	3534	1.24
PC-2B	3473	1.03
PC-3A	1691	1.89
PC-3B	1128	0.604
D1-2A	6945	1.37
D1-2B	6285	2.29



Regression Analysis
SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.893339485
R Square	0.798055435
Adjusted R Square	0.79109183
Standard Error	14203.43732
Observations	31

H_0 = PCDD/F not correlated to Aroclor 1268
H_A = PCDD/F correlated to Aroclor 1268
$p<0.05$
Status: PCDD/F correlated to Aroclor 1268

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	23119892311	23119892311	114.6037659	1.37521E-11
Residual	29	5850391320	201737631.7		
Total	30	28970283631			

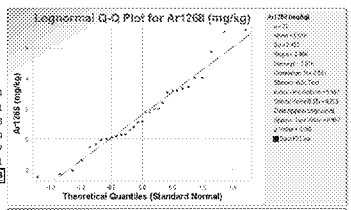
	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	11839.46177	2685.087013	4.409340075	0.000130408	6347.842219	17331.08132	6347.842219	17331.08132
Ar1268 (mg/kg)	89.18562551	8.330967078	10.70531484	1.37521E-11	72.1468847	106.2243663	72.1468847	106.2243663

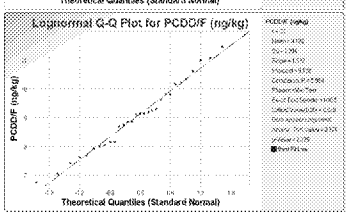
Spearman Correlation Analysis

Location	Log X	Log Y	$(\text{Log X})^2$	$(\text{Log Y})^2$	LOG X * LOG Y
36	1.7	4.4	3.028862291	19.64238427	7.713240372
61	3.1	5.2	9.696643201	26.54311177	16.0430385
68	2.5	4.8	6.342912465	23.11187261	12.10770766
1718	1.7	4.3	3.056161378	18.19052286	7.45608298
BR048	0.1	3.5	0.021353403	12.07119115	0.507701691
C-15	-1.0	4.0	1.008748662	16.2795209	-4.052399898
C-6	0.9	4.8	0.773817911	22.77428413	4.197953446
111	0.8	4.0	0.61674295	15.78441093	3.120083998
EPA-F2	3.1	5.0	9.454496144	24.73602903	15.29270058
GRID MARSH	0.8	3.8	0.61674295	14.26347177	2.965956111
117	1.0	3.3	1.084498725	11.08274061	3.466874394
110	-0.6	3.5	0.362476233	12.13895591	-2.097637484
100	0.0	2.9	0.001713354	8.598509567	0.121376662
101	-1.1	3.3	1.146143837	10.9783524	-3.547220171
102	-0.9	3.4	0.785096383	11.74990422	-3.037236788
D2-1A	0.5	4.0	0.231787005	16.16017141	1.935385679
D2-1B	0.5	3.9	0.257917586	15.5519681.7	2.002779592
EC-3A	1.4	4.0	1.92485053	15.76502022	5.508657508
EC-3B	1.3	4.5	1.807390586	20.20097731	6.042437935
EC-4A	1.5	4.4	2.129826433	19.52975653	6.449417934
EC-4B	0.9	4.0	0.781860517	15.92928417	3.529090301
LC-1A	-0.1	3.8	0.020182389	14.70702215	-0.544814503
LC-1B	0.0	4.2	0.000253541	17.53386518	-0.066674966
PC-1A	1.5	4.6	2.228333579	21.25487804	6.882075156
PC-1B	1.4	4.3	1.92978241	18.18077158	5.923253598
PC-2A	0.1	3.5	0.008727611	12.5905443	0.331489632
PC-2B	0.0	3.5	0.000164794	12.53685601	0.045453304
PC-3A	0.3	3.2	0.076431129	10.42091115	0.892458406
PC-3B	-0.2	3.1	0.047944822	9.315580021	-0.668306687
D1-2A	0.1	3.8	0.018692513	14.75839763	0.525234754
D1-2B	0.4	3.8	0.129481574	14.42733298	1.366774959

$$r = \frac{n(\sum xy) - (\sum x)(\sum y)}{\sqrt{[n\sum x^2 - (\sum x)^2][n\sum y^2 - (\sum y)^2]}}$$

∑LOG X	21.76095854
$\sum(\text{LOG X})^2$	49.59003691
∑LOG Y	123
$\sum(\text{LOG Y})^2$	496.808599
∑(LOG X x Log Y)	100.4129747
n	31
r	**0.778**



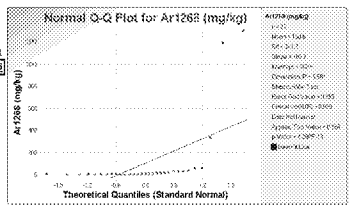


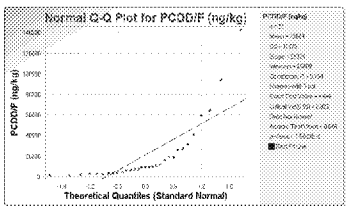
Pearson Correlation Analysis

Location	PCDD/F Rank	Ar1268 Rank	Rank Difference	Difference^2
36	7	5	2	4
61	1	1	0	0
68	3	3	0	0
1718	9	4	5	25
BR048	25	20	5	25
C-15	12	30	-18	324
C-6	4	13	-9	81
111	15	14.5	0.5	0.25
EPA-F2	2	2	0	0
GRID MARSH	21	14.5	6.5	42.25
117	27	11	16	256
110	24	28	-4	16
100	31	23	8	64
101	28	31	-3	9
102	26	29	-3	9
D2-1A	13	17	-4	16
D2-1B	17	16	1	1
EC-3A	16	9	7	49
EC-3B	6	10	-4	16
EC-4A	8	7	1	1
EC-4B	14	12	2	4
LC-1A	19	26	-7	49
LC-1B	11	25	-14	196
PC-1A	5	6	-1	1
PC-1B	10	8	2	4
PC-2A	22	22	0	0
PC-2B	23	24	-1	1
PC-3A	29	19	10	100
PC-3B	30	27	3	9
D1-2A	18	21	-3	9
D1-2B	20	18	2	4

$$r_s = 1 - \frac{6\sum d_i^2}{n(n^2-1)}$$

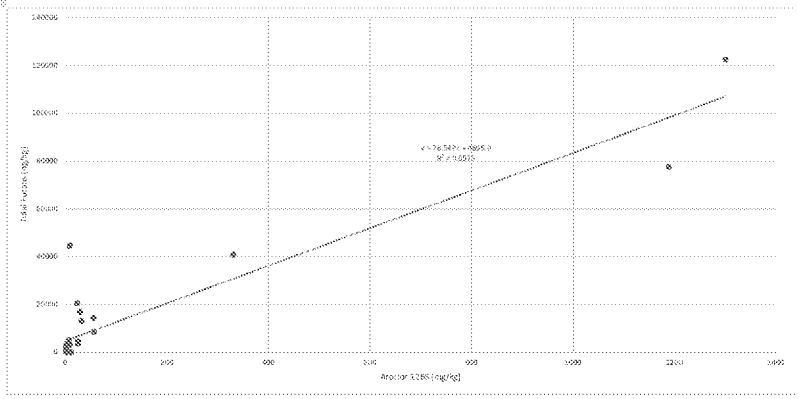
n=	31
r_s=	**0.795**





Case 3b: Co-location of Furan Mass and Aroclor 1268, Excluding Outliers (Original Distribution)

Location	Y- Furans (ng/kg)	X- Ar1268 (mg/kg)
36	14468	55
61	122400	1300
68	40850	330
1718	8750	56
BR048	391	1.4
C-15	1348	0.1
C-6	44710	8
111	5036	6
EPA-F2	77700	1188
GRID MARSH	3690	6
117	148	11.0
110	630	0.25
100	71	1.1
101	161	0.1
102	147	0.1
D2-1A	3831	3.0
D2-1B	3162	3
EC-3A	3810	24.4
EC-3B	20737	22
EC-4A	17065	29
EC-4B	3446	8
LC-1A	728	1
LC-1B	2958	1.0
PC-1A	13310	31.1
PC-1B	4611	25
PC-2A	649	1
PC-2B	207	1.0
PC-3A	316	1.9
PC-3B	206	0.6
D1-2A	565	1.37
D1-2B	600	2.29



Regression Analysis
SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.92591242
R Square	0.85731381
Adjusted R Square	0.852393597
Standard Error	10145.2033
Observations	31

H_0 = Furan mass not correlated to Aroclor 1268
H_A = Furan mass correlated to Aroclor 1268
$p<0.05$
Status: Furan mass correlated to Aroclor 1268

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	17934009093	17934009093	174.2432156	8.64297E-14
Residual	29	2984829349	102925150		
Total	30	20918838442			

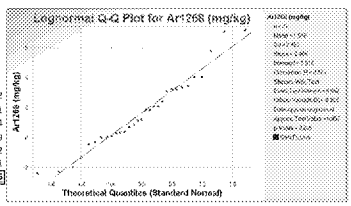
	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	4896.902459	1917.898675	2.553264426	0.016193616	974.3592385	8819.44568	974.3592385	8819.44568
Ar1268 (mg/kg)	78.54899847	5.950626794	13.2001218	8.64297E-14	66.37860016	90.71939678	66.37860016	90.71939678

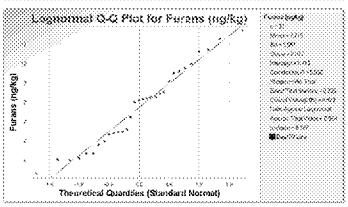
Pearson Correlation Analysis

Location	Log X	Log Y	$(\text{Log X})^2$	$(\text{Log Y})^2$	LOG X * LOG Y
36	1.7	4.2	3.028862291	17.30899887	7.240619722
61	3.1	5.1	9.696643201	25.88551971	15.84306311
68	2.5	4.6	6.342912465	21.26309213	11.61335146
1718	1.7	3.9	3.056161378	15.5394275	6.891371284
BR048	0.1	2.6	0.021353403	6.71938035	0.378789698
C-15	-1.0	3.1	1.008748662	9.794958832	-3.143350381
C-6	0.9	4.7	0.773817911	21.62626356	4.090817778
111	0.8	3.7	0.61674295	13.70549041	2.907363855
EPA-F2	3.1	4.9	9.454496144	23.91621774	15.03714695
GRID MARSH	0.8	3.6	0.61674295	12.72367703	2.801292221
117	1.0	2.2	1.084498725	4.70503774	2.258895179
110	-0.6	2.8	0.362476233	7.836307512	-1.685370947
100	0.0	1.8	0.001713354	3.415803012	0.07650151
101	-1.1	2.2	1.146143837	4.871258825	-2.362871829
102	-0.9	2.2	0.785096383	4.701767894	-1.921286279
D2-1A	0.5	3.6	0.231787005	12.84012598	1.725159221
D2-1B	0.5	3.5	0.257517586	12.24973306	1.777476184
EC-3A	1.4	3.6	1.92485053	12.82302368	4.96813888
EC-3B	1.3	4.3	1.807390586	18.6342954	5.803399873
EC-4A	1.5	4.2	2.129826433	17.91072367	6.176304131
EC-4B	0.9	3.5	0.781860517	12.51259934	3.127795932
LC-1A	-0.1	2.9	0.020182389	8.192478924	-0.406624884
LC-1B	0.0	3.5	0.000253541	12.04782829	-0.055268586
PC-1A	1.5	4.1	2.228333579	17.00884463	6.156409639
PC-1B	1.4	3.7	1.92978241	13.4233947	5.089619924
PC-2A	0.1	2.8	0.008727611	7.909849144	0.262743389
PC-2B	0.0	2.3	0.000164794	5.360801523	0.029722546
PC-3A	0.3	2.5	0.076431129	6.249809329	0.691143968
PC-3B	-0.2	2.3	0.047944822	5.355932006	-0.50674373
D1-2A	0.1	2.8	0.018692513	7.571654473	0.376209055
D1-2B	0.4	2.8	0.129481574	7.719732632	0.999781544

$$r = \frac{n\sum xy - (\sum x)(\sum y)}{\sqrt{[n\sum x^2 - (\sum x)^2][n\sum y^2 - (\sum y)^2]}}$$

∑LOG X	22
$\sum(\text{LOG X})^2$	49.59003691
∑LOG Y	104
$\sum(\text{LOG Y})^2$	371.8240279
∑(LOG X x Log Y)	96.24160042
n	31
r	**0.816**



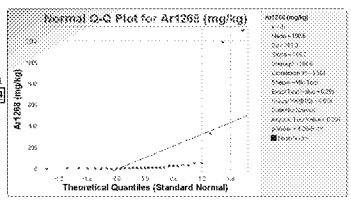


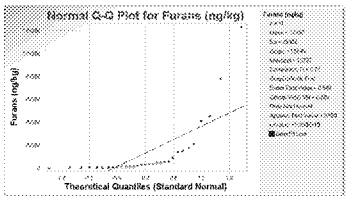
Spearman Correlation Analysis

Location	Aroclor 1268 Rank	Furans Rank	Rank Difference	Difference^2
36	5	7	-2	4
61	1	1	0	0
68	3	4	-1	1
1718	4	9	-5	25
BR048	20	24	-4	16
C-15	30	18	12	144
C-6	13	3	10	100
111	14.5	10	4.5	20.25
EPA-F2	2	2	0	0
GRID MARSH	14.5	14	0.5	0.25
117	11	29	-18	324
110	28	21	7	49
100	23	31	-8	64
101	31	28	3	9
102	29	30	-1	1
D2-1A	17	12	5	25
D2-1B	16	16	0	0
EC-3A	9	13	-4	16
EC-3B	10	5	5	25
EC-4A	7	6	1	1
EC-4B	12	15	-3	9
LC-1A	26	19	7	49
LC-1B	25	17	8	64
PC-1A	6	8	-2	4
PC-1B	8	11	-3	9
PC-2A	22	20	2	4
PC-2B	24	26	-2	4
PC-3A	19	25	-6	36
PC-3B	27	27	0	0
D1-2A	21	23	-2	4
D1-2B	18	22	-4	16

$$r_s = 1 - \frac{6\sum d_i^2}{n(n^2-1)}$$

n=	31
r_s=	**0.794**





APPENDIX E
Calculation for 95% UCL (ProUCL Input and Output)

PCDD/F TEQ in OU1 Sediment

Notes:
*TEQ results in ng/kg

Location	Parameter	val	D_val
D1-1A	TEQ	42.0	1
D1-1B	TEQ	51.5	1
D1-2A	TEQ	26.9	1
D1-2B	TEQ	27.6	1
D2-1A	TEQ	118.7	1
D2-1B	TEQ	71.0	1
EC-1A	TEQ	39.9	1
EC-1B	TEQ	39.3	1
EC-2A	TEQ	80.8	1
EC-2B	TEQ	14.1	1
EC-3A	TEQ	135.0	1
EC-3B	TEQ	863.3	1
EC-4A	TEQ	735.6	1
EC-4B	TEQ	123.9	1
LC-1A	TEQ	23.3	1
LC-1B	TEQ	112.4	1
MC-1A	TEQ	68.0	1
MC-1B	TEQ	50.4	1
MC-2A	TEQ	53.2	1
MC-2B	TEQ	69.2	1
MC-3A	TEQ	41.4	1
MC-3B	TEQ	56.1	1
PC-1A	TEQ	381.0	1
PC-1B	TEQ	121.3	1
PC-2A	TEQ	19.8	1
PC-2B	TEQ	11.6	1
PC-3A	TEQ	11.0	1
PC-3B	TEQ	6.9	1

UCL Statistics for Data Sets with Non-Detects

User Selected Options	
Date/Time of Computation	ProUCL 5.17/13/2018 11:27:53 PM
From File	Book1.xls
Full Precision	OFF
Confidence Coefficient	95%
Number of Bootstrap Operations	2000

val

General Statistics

Total Number of Observations	28	Number of Distinct Observations	28
		Number of Missing Observations	0
Minimum	6.9	Mean	121.3
Maximum	863.3	Median	52.35
SD	205.2	Std. Error of Mean	38.77
Coefficient of Variation	1.692	Skewness	2.979

Normal GOF Test

Shapiro Wilk Test Statistic	0.526	**Shapiro Wilk GOF Test**
5% Shapiro Wilk Critical Value	0.924	Data Not Normal at 5% Significance Level
Lilliefors Test Statistic	0.366	**Lilliefors GOF Test**
5% Lilliefors Critical Value	0.164	Data Not Normal at 5% Significance Level

Data Not Normal at 5% Significance Level

Assuming Normal Distribution

95% Normal UCL		**95% UCLs (Adjusted for Skewness)**	
95% Student's-t UCL	187.3	95% Adjusted-CLT UCL (Chen-1995)	208.4
		95% Modified-t UCL (Johnson-1978)	190.9

Gamma GOF Test

A-D Test Statistic	1.696	**Anderson-Darling Gamma GOF Test**
5% A-D Critical Value	0.783	Data Not Gamma Distributed at 5% Significance Level
K-S Test Statistic	0.211	**Kolmogorov-Smirnov Gamma GOF Test**
5% K-S Critical Value	0.172	Data Not Gamma Distributed at 5% Significance Level

Data Not Gamma Distributed at 5% Significance Level

Gamma Statistics

k hat (MLE)	0.791	k star (bias corrected MLE)	0.73
Theta hat (MLE)	153.4	Theta star (bias corrected MLE)	166.2
nu hat (MLE)	44.27	nu star (bias corrected)	40.86
MLE Mean (bias corrected)	121.3	MLE Sd (bias corrected)	142
		Approximate Chi Square Value (0.05)	27.21
Adjusted Level of Significance	0.0404	Adjusted Chi Square Value	26.52

Assuming Gamma Distribution

95% Approximate Gamma UCL (use when n>=50))	182.1	95% Adjusted Gamma UCL (use when n<50)	186.8

Lognormal GOF Test

Shapiro Wilk Test Statistic	0.955	**Shapiro Wilk Lognormal GOF Test**
5% Shapiro Wilk Critical Value	0.924	Data appear Lognormal at 5% Significance Level
Lilliefors Test Statistic	0.121	**Lilliefors Lognormal GOF Test**
5% Lilliefors Critical Value	0.164	Data appear Lognormal at 5% Significance Level

Data appear Lognormal at 5% Significance Level

Lognormal Statistics

Minimum of Logged Data	1.932	Mean of logged Data	4.046
Maximum of Logged Data	6.761	SD of logged Data	1.152

Assuming Lognormal Distribution

95% H-UCL	199.7	90% Chebyshev (MVUE) UCL	189.3
95% Chebyshev (MVUE) UCL	226.7	97.5% Chebyshev (MVUE) UCL	278.4
99% Chebyshev (MVUE) UCL	380.1		

Nonparametric Distribution Free UCL Statistics

Data appear to follow a Discernible Distribution at 5% Significance Level

Nonparametric Distribution Free UCLs

95% CLT UCL	185	95% Jackknife UCL	187.3
95% Standard Bootstrap UCL	183	95% Bootstrap-t UCL	306.2
95% Hall's Bootstrap UCL	389.2	95% Percentile Bootstrap UCL	189.5
95% BCA Bootstrap UCL	208.9		
90% Chebyshev(Mean, Sd) UCL	237.6	95% Chebyshev(Mean, Sd) UCL	290.3
97.5% Chebyshev(Mean, Sd) UCL	363.4	99% Chebyshev(Mean, Sd) UCL	507

Suggested UCL to Use

95% H-UCL	199.7

Note: Suggestions regarding the selection of a 95% UCL are provided to help the user to select the most appropriate 95% UCL.
Recommendations are based upon data size, data distribution, and skewness.
These recommendations are based upon the results of the simulation studies summarized in Singh, Maichle, and Lee (2006).
However, simulations results will not cover all Real World data sets; for additional insight the user may want to consult a statistician.

ProUCL computes and outputs H-statistic based UCLs for historical reasons only.
H-statistic often results in unstable (both high and low) values of UCL95 as shown in examples in the Technical Guide.
It is therefore recommended to avoid the use of H-statistic based 95% UCLs.
Use of nonparametric methods are preferred to compute UCL95 for skewed data sets which do not follow a gamma distribution.