Relationship and Translation of PCB Aroclor and Congener Data – How Useful Are They?

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Introduction

Many sites in the USA are contaminated with polychlorinated biphenyls (PCBs) (EPA, 2005; Asher et al., 2007; Breault, 2014). Chemical analysis to determine total PCBs traditionally used Aroclor based analytical methods that can be problematic due to many reasons including identification and fate and transport issues (Leidos, 2016). More recent methods using high resolution gas chromatography/mass spectrometry (HRGC/MS) can analyze 209 PCB congeners and provide better detection and quantification of total PCBs. Therefore, many new investigations are using congener analysis in addition to old Aroclor data. This poster looks into the relationship between paired Aroclor and congener data, shows methods to translate these data from one to another, and discusses the usefulness of such transformation.

Methodology

WA State Department of Ecology (Ecology) collected 30 paired samples of storm drain solids from the Lower Duwamish Waterway (LDW) Superfund site source control area located in southern Seattle, Washington. The samples were analyzed for both PCB Aroclors (EPA method 8082A) and 209 PCB congeners (EPA method 1668C). Total PCBs both as sum of Aroclors and sum of congeners were calculated using traditional approach. The results were plotted to see visual comparison between the totals calculated from each method. Statistical analysis were performed using Minitab software to find regression equations, calculate correlation coefficients, and perform paired t-test.
Congener data were then used to calculate individual Aroclors based on a method used in National Environmental Laboratory Accreditation Program (NELAP) accreditation (Leidos, 2016).

The following formulas were used:
Aroclor 1016 = ∑ (PCBs 8, 18/30, 31, 28/20) x 2.7
Aroclor 1248 = ∑ (PCBs 44/47/65, 49/69, 66) × 6.1
Aroclor 1254= ∑ (PCBs 83/99, 86/87/97/108/119/125) × 8.0
Aroclor 1260= ∑ (PCBs 170, 180/193, 183/185) × 5.0

These calculated Aroclor values were then compared with laboratory measured values and Pearson's correlation coefficients (r) were used to observe any statistical correlations.

Results

A moderate level of correlation (Pearson's r = 0.52 with a p-value of 0.003) was found between the sum of Aroclors and sum of congeners for samples collected at the LDW site (Figure 1). In addition, total PCBs measured by the Aroclor method were lower when compared to total PCBs by the congener method as interpreted from paired t-test results (p-value = 0.038) and regression equation (Total PCB Congeners = 669 + 1.26 x Total PCB Aroclors). Other investigations show similar or better correlation but relationship was different (Ecology, 2014). Therefore, a site specific relationship is necessary to use Aroclor data in conjunction with congener data.

Analytically measured Aroclors 1016, 1248, 1254 and 1260 were plotted with calculated values from the method 1668C congener data (Figure 2.a – 2.d). Table 1 shows the correlation between measured and calculated values of these Aroclors using Pearson's r and corresponding p-value statistic. Statistical analysis shows that correlation between measured and calculated may or may not exist. A low level correlation exists for Aroclor 1260, which was detected at the highest percentage (70%). Other Aroclors that were not detected frequently (10-23%), show mixed correlation (no to very high). Therefore, while it is possible to translate method 1668 congener data into individual Aroclors, such translation may or may not lead to meaningful correlation. This may be related with uncertainty and limitations of measuring environmentally weathered PCB Aroclors in the laboratory (Leidos, 2016).

Table 2 depicts the effects of substitution of non-detect analytical results as zero, half the reporting limit, and reporting limit on correlation coefficient and p-value. No significant differences in the values were observed when such substitutions occurred.

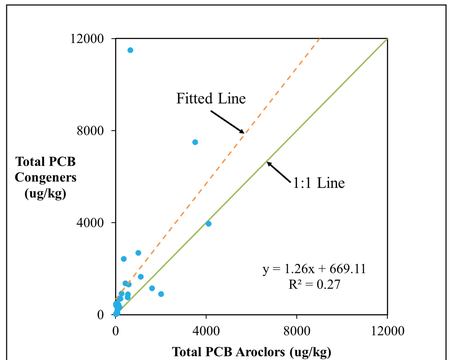

Figure 1: Paired sampling results for total Aroclors versus total 209 congeners

Table 1: Correlation between measured and calculated Aroclors

Aroclor	Frequency of Detection	Pearson's r	p-value	Interpretation @ 95% Significance Level
Aroclor 1260	21/30	0.42	0.02	Low correlation
Aroclor 1254	7/30	0.30	0.11	No correlation
Aroclor 1248	3/30	0.93	0.00	Very high correlation
Aroclor 1016	3/30	0.12	0.54	No correlation

Table 2: Effects of substitution for non-detect Aroclors

Aroclor	Pearson's r			p-value		
	U=0	U=1/2 RL	U=RL	U=0	U=1/2 RL	U=RL
Aroclor 1260	0.42	0.42	0.42	0.02	0.02	0.02
Aroclor 1254		0.30	0.34	0.19	0.11	0.06
Aroclor 1248	0.92	0.93	0.94	0.00	0.00	0.00
Aroclor 1016	0.13	0.12	0.08	0.47	0.54	0.67

U = non-detect; RL = method reporting limit

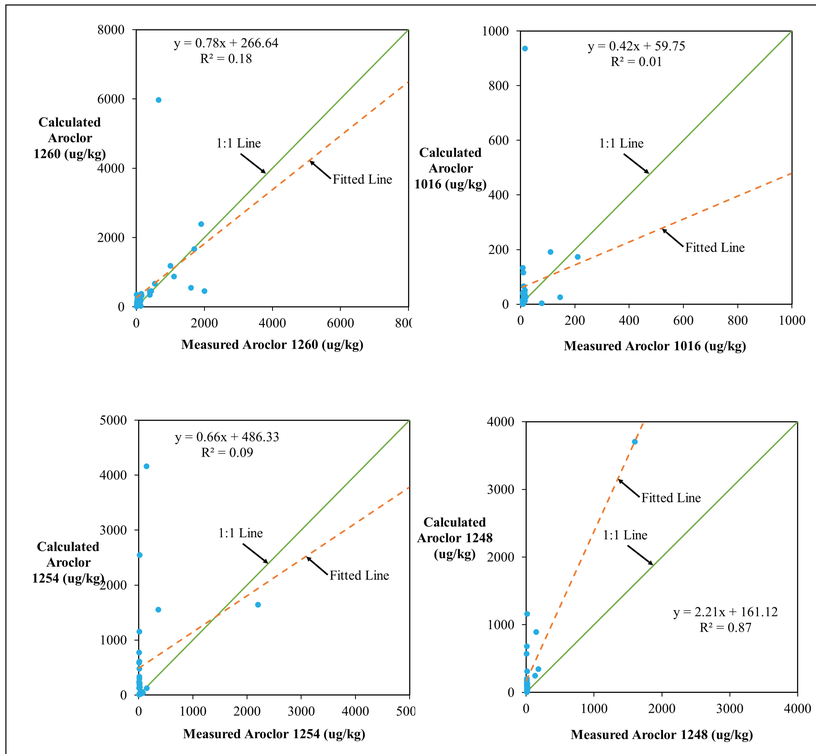

Figure 2.a – 2.d: Comparison of EPA method 8082A measured Aroclors and calculated Aroclors from 209 congeners using EPA method 1668C

Conclusions

- Statistical correlation between total PCB Aroclors and total PCB congeners may exist, however, a site specific relationship between them is necessary.
- Calculated PCB Aroclors from congener data may or may not have statistical correlation with measured Aroclor data.This may be associated with difficulties in measuring PCB Aroclors in the laboratory when environmental samples are subject to weathering.
- When using older Aroclor data with newer congener data, site specific information and knowledge about PCB analytical methods are necessary.

Limitations and Future Work

Several PCB Aroclors and congeners were below method detection limits that created difficulty in calculating total PCBs and comparing measured versus calculated values. Non-detected PCB congeners or Aroclors were assumed to be zero. When all Aroclors were non-detect in a sample, the highest method reporting limit was assumed as total PCBs. Substitution of non-detect analytical results as zero, half the reporting limit, and reporting limit were also explored in this study. This may not be a good method when statistical inferences are sought. In future, survival analysis methods, such as, Kaplan-Meier (K-M), MLE (Maximum Likelihood Estimation), Regression on Order Statistics (ROS) may be used to handle non-detect analytical results.

References

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