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Short Communication

A STATISTICAL BIAS IN THE DERIVATION OF HARDNESS-DEPENDENT METALS CRITERIA

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Abstract – Log-transformed values of lethal effect and hardness are often employed to predict metal effects. For example, they are used to develop water quality criteria. A statistical bias encountered with backtransformed, least-squares regression models can compromise the accuracy of associated predictions. A description and method of estimating this bias are discussed herein. In a selected data set, the bias was as high as 57%.

Keywords – Statistics Metal Toxicity Criteria Bias Hardness

INTRODUCTION

The Clean Water Act mandates development of ambient water quality criteria by the U.S. Environmental Protection Agency (EPA) [1]. These criteria (or state-specific ambient criteria) are adopted as part of state water quality standards and are often implemented in the derivation of effluent limitations. As our understanding of and ability to estimate contaminant effects continue to be refined, ambient criteria are periodically updated to reflect recent toxicological data.

Procedures for estimating effects of metals are clearly outlined in the current "Quality Criteria for Water 1986" [1]. Desiring to further refine metals criteria, I present a simple analysis that indicates a statistical bias in the present methods. This bias appears during the incorporation of hardness into estimation of final acute values (FAV) or final chronic values (FCV).

When a relationship exists between toxic end point (i.e., effect) and a water quality variable, this association is incorporated into estimations of effect [1]. Such a clear relationship has been documented between toxic effects of several metals and hardness [2,3]. "Because the best documented relationship is that between hardness and acute toxicity of metals in fresh water and a log–log relationship fits these data, geometric means and natural logarithms of both toxicity and water quality are used [to illustrate incorporation of water quality effects into criteria]. . . . For relationships based on other water quality characteristics such as pH, temperature, or salinity, no transformation or a different transformation might fit the data better" [4]. In general terms, least-squares regression is used for log-transformed values of hardness and toxicity and, after backtransformation to arithmetic units, a final acute (or chronic) equation (FAE or FCE) is generated. Unlike predicted FAV (or FCV) values generated by least-squares regression for other toxicant-water quality relationships that do not require log-transformation and backtransformation, predicted values from metal FAEs will be biased downward. The predicted concentrations having an impact (FAV or FCV) will be lower than statistically unbiased, predicted values. The extent of the bias depends on the residual distribution and error variance of the log–log regression model as detailed below.

BIAS IN PREDICTED TOXIC EFFECT

The following discussion is based primarily on material from Beauchamp and Olson [5] and is supplemented with material from Sprugel [6] and Koch and Smillie [7]. An identical explanation relative to a similar group of relationships involving animal size-specific, metal bioaccumulation is given in Newman and Heagler [8]. To simplify discussion, the normalization and averaging procedures used in formulating the FAE [1, Appendix A; 4] will be omitted here. Instead, simple, least-squares regression techniques will be used to illustrate the problem.

Similar procedures are used in many fields for fitting data to a power relationship. The relationship is transformed to a linear one by taking the logarithms of the X and Y variables (hardness and toxic effect in this case). Least-squares regression is then used to generate the following equation:

$$\log Y = b \log X + \log a \tag{1}$$

where b and $\log a$ are the regression slope and intercepts, respectively.

The regression model of the log-transformed variables also has an associated error term such that the equation describing the model is actually the following:

$$\log Y = b \log X + \log a + \epsilon \tag{2}$$

where ϵ is the random error of the model.

Often, the results of the regression are back-transformed as follows, without consideration of this error term (ϵ):

$$Y = aX^b. \tag{3}$$

Consequently, when the model is used for predictions, it produces biased estimates of Y. The back-transformed model is better described by the following:

$$Y_p = aX^b e^\epsilon, \tag{4}$$

where Y_p is the predicted value of Y.

Unless $\epsilon = 0$ (perfect fit of the data to the model), the predicted Y (FAV or FCV in the present discussion) will be biased. Assuming a normal distribution for the model residuals, the bias can be estimated as follows:

$$\text{estimate of bias} = e^{\sigma^2/2} \tag{5}$$

where σ^2 is the error variance of the log–log regression model.

An unbiased estimate of the Y_p would be calculated by multiplying the biased estimate by the term on the right side of Equation 5. If a normal distribution cannot be assumed for the residuals, then a nonparametric, "smearing estimate of bias" is recommended by Koch and Smillie [7].

EXAMPLES

Table 1 summarizes results from regression analysis of selected data sets. These examples were taken from tables in Canadian [9] and U.S. [10–12] criteria documents for cadmium, copper, and zinc. Only the most complete data sets within these tables were used for bias illustration. When observation pairs were omitted in calculations in the criteria documents, they were omitted from regression analysis in the present treatment also. As residual analyses for all data sets showed no significant deviations from the assumption of normality ($\alpha = 0.05$, Shapiro–Wilk W statistic), Equation 5 was used to estimate the associated bias; the error mean square divided by 2 was used as the exponent for the base e to estimate the bias. The bias estimates were converted to percentages for ease of comparison of unbiased predictions to biased predictions.

The biases estimated for half of the selected examples were minor. For example, the estimated bias for copper effects on Cypriniformes was 3%. However, bias estimates for four species examined were 20% or greater, with one species (bluegill) having a bias estimate of 57% (Table 1). Although these examples are not sufficient to estimate the magnitudes of biases in predictions developed from published regression/analysis of covariance models presented in water quality criteria documents, they do suggest that these biases can be significant. Estimation of such bias (and correction, if appropriate) would add defensibility to national or site-specific criteria.

CONCLUSION

The median Y_p, not the mean Y_p, will be generated from the FAE (or FCE) if this transformation bias is ignored. One could argue that the median predicted FAV (or FCV) is adequate and that the mean predicted FAV (or FCV) is not necessary. However, the regression techniques described for similar adjustments made for other water quality variables on toxic effects of other toxicants (see quote from [4] in Introduction) will result in mean predicted FAVs (or FCVs). Consequently, an inconsistency arises in that mean predicted values are used for some toxicants but median predicted values are used for metals. It is recommended that either (a) the bias in the metals criteria be corrected (if necessary) by re-analysis of associated regression (or covariance) models or (b) it be clearly stated with justification that median predicted FAVs (or FCVs) are used for metals but not for other toxicants. To correct for this statistical bias, the author recommends that the EPA perform adjusted calculations by re-analysis of associated regression (or covariance) models when ambient water quality criteria are updated.

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Table 1. Examples of the statistical bias: Copper, cadmium and zinc toxicity (LC50 or EC50, mg/L) vs. hardness (mg/L as $CaCO_3$)

Data	N	ln a	ln b	Model mean square ($d.f. = 1$)	Error mean square ($d.f. = N - 2$)	r^2	F value	Probability $>F$	Bias estimated[a]
Cu									
Cypriniformes [9]	18	−7.04	1.20	33.44	0.0795	0.963	420.54	0.0001	4
Perciformes [9]	11	−2.00	0.49	1.59	0.0568	0.757	28.08	0.0005	3
Salmon-like A[b] [9]	16	−6.64	1.10	14.09	0.0481	0.954	292.95	0.0001	2
Salmon-like B[c] [9]	5	−6.59	0.80	4.18	0.0642	0.956	65.18	0.0040	3
Fathead minnow[c] [10] (*Pimephales promelas*)	27	−7.13	1.21	41.15	0.2628	0.862	156.60	0.0001	14
Bluegill[d] [10] (*Lepomis macrochirus*)	15	−2.95	0.78	10.47	0.8991	0.472	11.64	0.0046	57
Guppy[d] [10] (*Poecilia reticulata*)	6	−7.27	1.23	6.85	0.4244	0.801	16.14	0.0159	24
Cd									
Daphnia magna [11]	5	−9.11	1.19	1.84	0.0524	0.921	35.11	0.0096	3
Zn									
Fathead minnow [12] (>1 g) (*P. promelas*)	29	−1.93	0.91	16.30	0.3230	0.65	50.45	0.0001	18
Juvenile brook trout [12] (*Salvelinus fontinalis*)	6	−2.43	0.82	1.80	0.0429	0.91	41.89	0.0029	2
Daphnia magna [12]	7	−6.65	1.25	3.51	0.3589	0.66	9.77	0.0261	20
Rainbow trout [12] (*Salmo gairdneri*)	25	−3.72	0.87	25.75	0.4442	0.72	57.98	0.0001	25

Relationships from selected criteria documents.
[a]Expressed as percentage [100 − (bias from Eqn. 5·100)].
[b]Trout, Atlantic salmon, and two species of Pacific salmon (i.e., *Oncorhynchus nerka* and *O. gorbuscha*), as delineated in reference [9].
[c]Two species of Pacific salmon (i.e., *O. kisutch* and *O. tshawytscha*), as delineated in reference [9].
[d]Data selected as per discussion in reference [10].

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