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A field-based model of the relationship between extirpation of salt-intolerant benthic invertebrates and background conductivity

Susan M. Cormier^{a,*}, Lei Zheng^{b,1}, Colleen M. Flaherty^c

^aU.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, 26 Martin Luther King Dr. W, Cincinnati, OH 45268, USA

^bTetra Tech, 10711 Red Run Blvd., Suite 105, Owings Mills, MD 21117, USA

^cU.S. Environmental Protection Agency, Office of Water, Office of Science and Technology, Health and Ecological Criteria Division, 1200 Pennsylvania Avenue, N. W., Washington, DC 20460, USA

Abstract

Field-collected measures of dissolved salts and occurrences of aquatic invertebrates have been used to develop protective levels. However, sufficiently large field data sets of exposures and biota are often not available. Therefore, a model was developed to predict the exposure extirpating 5% of benthic invertebrate genera using only measures of specific conductivity (SC) as the independent variable. The model is based on 3 assumptions: (1) a genus will rarely occur where the background exceeds its upper physiological limit; (2) the lowest possible tolerance limit of a genus in a region is defined by the natural background; and (3) as a result, there will be a regular association between natural background SC and the SC at which salt-intolerant genera are present. Three steps were used to develop the model. First, background SC was characterized as the 25th centile of sampled sites for each of 24 areas in the United States with streams dominated by bicarbonate and sulfate ions. Second, the extirpation concentration (XC_{95}), an estimate of the upper tolerance limit with respect to SC, was calculated for genera in 24 data sets. Next, the lower 5th centile of each set of XC_{95} values (XCD_{05}) was identified for the most salt-intolerant members in each data set. Finally, the relationship between the 24 background SC and the 24 XCD_{05} values was empirically modeled to develop a background-to-criterion model. The least squares regression of XCD_{05} values on log background SC ($\log Y = 0.658\log X + 1.071$) yields a strong linear relationship ($r = 0.93$). The regression model makes it possible to use SC background to predict the SC likely to extirpate the most salt-intolerant genera in an area. The results also suggest that species distribute along natural background gradients of SC and that this relationship can be used to develop criteria for ionic concentration.

Graphical Abstract

*Corresponding author. cormier.susan@epa.gov (S.M. Cormier).

¹Present address: Noblis, 2275-J Rolling Run Dr., Woodlawn, MD 21244, USA.

Keywords

Niche; Background-to-criterion model; Water quality criteria; Salinization; Stream

1. Introduction

Salinization of fresh water is recognized as a threat to biodiversity and ecosystem function (Environment Canada and Health Canada, 2001; Zielinski et al., 2001; Higgins and Wilde, 2005; Kaushal et al., 2005, 2013, 2018; Zalizniak et al., 2006; Findlay and Kelly, 2011; Gillis, 2011; Karatayev et al., 2012; Cañedo-Argüelles et al., 2013; Vander Laan et al., 2013; Pond et al., 2014; Dunlop et al., 2015; Clements and Kotalik, 2016; Zhao et al., 2016).

One way to reduce salinization is to implement limits on loadings of ionic minerals to water. There are several challenges in developing limits or water quality criteria for salts. First, the ionic mixtures of salts vary and have differing toxicities which also differ by species (Zalizniak et al., 2006; Dunlop et al., 2015; Mount et al., 2016). Second, the effects of ionic toxicity may not be readily measured with conventional toxicity tests (Wood-Eggenschwiler and Barlocher, 1983; Micieli et al., 2012; Olson, 2012; Clements and Kotalik, 2016; Olson and Hawkins, 2017). Furthermore, a single benchmark is not appropriate for all locations because background specific conductivity (SC) varies naturally across the landscape (Griffith, 2014). One option is to derive a new benchmark by applying the U.S. Environmental Protection Agency's (U.S. EPA, 2011) field-based method to paired biological and SC data sets from the region of interest. The U.S. EPA field-based method estimates the upper tolerance for numerous taxa, the extirpation concentration for the 95th centile of occurrences of a species or genus (XC_{95}). Then the 5th centile of the distribution of XC_{95} values (XCD_{05}) is calculated which represents the exposure level expected to cause 5% of genera to be extirpated from a stream in a region. Although this has been performed for the Han River basin in China (Zhao et al., 2016) and in streams of Australia (van Dam personal communication), data sets sufficient to perform such analysis are often not available. Another option is to develop a model that estimates a benchmark for any region and that requires only the background SC for the region. Such a background-to-criterion (B-C) model is described here and is part of a draft aquatic life criterion method (U.S. EPA, 2016). The B-C model assumes that background SC in a region and the proportion of organisms extirpated by an increase in SC are related to one another and can provide a model for predicting a benchmark or criterion. These assumptions are tested in this manuscript.

It is well known that it is physiologically possible for aquatic organisms to thrive in low SC waters (Bos et al., 1996; Potapova and Charles, 2003; Potapova, 2005; U.S. EPA, 2011) with different mechanisms of ion regulation (Sutcliffe, 1962; Wichard et al., 1973; Komnick,

1977; Hille, 2001; Smith, 2001; Thorp and Covich, 2001; Marshall, 2002; Nelson and Cox, 2005; Evans, 2008; Wood and Shuttleworth, 2008; Bradley, 2009; Griffith, 2017). Thus, the lowest conductivity habitats are likely to be occupied by benthic invertebrates in any natural SC regime. However, it is likely that the ability to survive in dilute waters evolved at the expense of other traits that are advantageous at higher salt concentrations (Griffith, 2017; Kefford et al., 2016; Olson and Hawkins, 2017). Therefore, in habitats of higher SC, the most salt-intolerant species would be physiologically or competitively disadvantaged. Thus, different species would be found in different niches partly defined by the ability to tolerate ionic stress. This would create a regular pattern of salt-tolerance niches in which the least salt-tolerant species of a SC niche would be more salt-tolerant than a lower SC niche. In other words, the least salt-tolerant species would not occur in habitats with a higher natural background SC, but species tolerant of that SC range would occur. If this is true, then there should be an inherent and regular association between background SC and a proportion of taxa extirpated at a higher SC level. The objective of this study was to develop a model of this relationship that could be used to predict the change in SC level that would extirpate 5% of taxa using only the background SC for the location or area as an independent variable.

2. Methods

To develop a model of the relationship between background SC and the SC level that extirpates 5% of benthic invertebrate genera, 24 distinct data sets were obtained from different state agencies in the USA. These data sets had a wide range of background SC with a dominant ion mixture of HCO_3^- and SO_4^{2-} (mg/L) characteristic of the ion composition of fresh water in most of the study area (Griffith, 2014). Cl^- was typically not a dominant ion. Ca^{2+} was the dominant cation. Na^+ was less frequently measured and reported by the states that assembled these data sets, but where it was measured it was usually not dominant. These data were used to estimate the extirpation concentrations (XC) of freshwater aquatic benthic invertebrate genera (U.S. EPA, 2011; Cormier and Suter II, 2013).

The operational estimate of an XC described by this method is the SC at the 95th centile of the occurrences of each genus (XC_{95}) in each region (U.S. EPA, 2011; Cormier and Suter II, 2013, Cormier et al., 2013, 2017). The XC_{95} value represents an exposure level above which only 5% of occurrences of that genus are observed. Next, 24 cumulative frequency distributions of genus XC_{95} values (extirpation concentration distributions [XCDs]) were constructed from each of the 24 sets of XC_{95} values. An XCD is a type of species sensitivity distribution (Posthuma et al., 2001) that describes extirpation rather than sensitivity. From each of the 24 XCDs, the SC at which 5% of genera were likely to be extirpated was identified, that is, a SC level for 5% of taxa's XC_{95} values, an XCD_{05} . The 5% effect threshold was selected to be consistent with U.S. EPA's guidelines for aquatic life criteria developed using laboratory tests (Stephan et al., 1985). The 24 XCD_{05} values were regressed against the 25th centile of SC of each data set to develop a B-C model.

To develop the model, the background of each data set was estimated. It was not necessary to determine background in the absence of anthropogenic influence for model building. This is because the model depends on the organisms in each data set responding to their environment as conditions currently exist, not whether the ionic concentration is

anthropogenic or natural background. The 25th centile SC was used to characterize “background” for a data set of mixed exposures that are not reference sites because the 25th centile is a conventional cut-off value for background in nonreference data sets (U.S. EPA, 2000; sensu Stoddard et al., 2006), but it does not necessarily represent natural background (i.e. no anthropogenic alteration). The 75th centile of best available reference sites has been shown to be comparable to the 25th centile of a mixed probability data set (U.S. EPA, 2011).

2.1. Data sets

Ecoregions are geographic areas with similar vegetation, animal life, geology, physiography, climate, soils, water quality, and hydrology (Omernik, 1987). State data sets from 48 Level III ecoregions in the conterminous United States were considered. There were five requirements for inclusion of a data set in the B-C model.

- A minimum of 200 sites sampled for both biology and SC. A minimum of 500 sites is recommended to derive a stand-alone, region-specific criterion (U.S. EPA, 2016). However, less precise values are adequate as a group to represent a general relationship between the occurrence of salt-intolerant genera and regional SC levels represented in the data set.
- Taxonomic identification to genus of all individuals or a minimum sample or subsample of at least 100 individuals.
- Information about the ionic composition of streams in the region indicating that $[\text{HCO}^-] + [\text{SO}_4^{2-}] - [\text{Cl}^-]$ in mg/L.
- 5% of XC_{95} values are unambiguous based on a generalized additive model as described in U.S. EPA (2011). If the mean fitted curve of the generalized additive model at maximum SC is approximately equal to 0 (defined as $> 1\%$ of the maximum modeled probability), then an XC_{95} is unambiguous and clearly defined.

The 24 data sets that met all those data set requirements for estimating XC_{95} values are listed in Table 1. Two state data sets were available from the same Southeastern Coastal Plains, Level III Ecoregion 65, separated by > 1000 km, one in the state of Maryland and one in Mississippi. Background SC was different in the two data sets (99 and 38 $\mu\text{S}/\text{cm}$, respectively), so both sets were retained as distinct data sets. Any sites with a pH of < 6 were removed from all data sets prior to analysis to avoid potential effects of acidification. If pH was not measured, the data were retained.

2.2. Development of individual XC_{95} and XCD_{05} values

Prior to developing the B-C model, XCD_{05} values were derived for each of the 24 data sets (U.S. EPA, 2011; Cormier and Suter II, 2013) (Fig. 1) from XC_{95} values calculated for each genus occurring in 25 samples. Occurrences of a genus were weighted to adjust for uneven sampling throughout the sampled range of SC in each data set thus correcting for any potential bias from the unequal distribution of sampling of sites across the range of conductivity (Cormier and Suter II, 2013). For a detailed example and spreadsheet tool to calculate a weighted XC_{95} and an XCD_{05} , see Cormier et al. (2017).

Sets of XC_{95} values were ranked from lowest to highest SC, and the XCD_{05} was estimated by interpolation at the 5th centile of all genera in each data set. More than 2700 XC_{95} values were evaluated for reliability characterized as unambiguous, approximate, or greater than the evaluated range. Unambiguous means that the XC_{95} is clearly defined, that is, the occurrence of the genus decreases with increasing SC and the tested range was wide enough to measure the upper tolerance limit, i.e. XC_{95} . The evaluation of reliability of the XC_{95} values was based on whether the probability of observing a genus was near zero at sites with conductivity > the genus' XC_{95} value. The process for evaluating the XC_{95} values is based on inspection of scatter plots and generalized additive models of the probability of observing each genus in each data set (Cormier and Suter II, 2013; Cormier et al., 2013; U.S. EPA, 2011).

Unambiguous XC_{95} values are needed in the lower 5th centile of the XC_{95} distribution. If all the XC_{95} values were ambiguous, the 5th centile of the XC_{95} distribution would be undefined. However, all the XC_{95} values do not need to be defined because only the count of all the XC_{95} values is used to identify the 5th centile of the distribution, not the XC_{95} values themselves. Four data sets were identified in which < 5% of XC_{95} values were unambiguous (Fig. 1), so they were not used in model development. The number of genera and the proportion of unambiguous XC_{95} values for each data set are listed in Table 1.

2.3. Development and validation of regression model

The B-C regression model was developed using the paired background SC and XCD_{05} values listed in Table 1. The upper bound of background was identified as the 25th centile of the cumulative frequency distribution of SC in each data set (U.S. EPA, 2011). In areas with anthropogenically elevated background SC, the 25th centile SC would not represent natural background, but the background experienced by the genera in the data set. Therefore, the XCD_{05} for any data set likely represents a community of organisms that is capable of populating that sampled background SC irrespective of any deviation from natural background. A linear least squares regression was used to develop the B-C model using the log10 of background SC as the independent variable and the log of XCD_{05} as the dependent variable. The 50% prediction interval (PI) was calculated.

Non-linear model assumptions and potential spatial autocorrelation were evaluated using several tests. Heteroscedasticity was checked with a side-by-side plot of residuals against the fitted values. No pattern was evident, and the residuals were equally distributed between positive and negative values. Normality was checked by plotting the ordered residuals against the z-score. There was a slight deviation from the 1:1 line, but within reasonable practical limits. Potential spatial autocorrelation was evaluated by identifying geographic coordinates of the state ecoregion polygons (one for each of the 24 data sets) and calculating the Moran's I using the "ape" package in R and confirmed using ArcMap. The null hypothesis is that there is zero spatial autocorrelation. The calculated (observed) Moran's I is -0.02, the expected value is -0.04, and the p-value is 0.86. So, the null hypothesis is not rejected, that is, spatial autocorrelation is not evident. The results of these tests show that the model assumptions are met. The scatter of data around the line is normally-distributed, the variability in the predictions are the same along the range of tested x-values and across the

geographic range, and the residuals are independent, that is, they occur, randomly above and below the regression line.

Validation of the B-C model was performed using a “leave-one-out cross-validation” (LOOCV) procedure (James et al., 2013). This procedure involves reserving one ecoregional data pair for validation and rederiving the B-C model with the remaining 23 ecoregional pairs to produce a test model (left branch in Fig. 2). An XCD_{05} is calculated from each LOOCV test model using the observed background SC from the removed data pair. The squared error (SE) is calculated by subtracting the observed XCD_{05} from the XCD_{05} generated by the LOOCV test regression model and then squaring the difference. This was repeated using all 24 state data sets to generate 24 SE values. A small SE indicates that the predicted XCD_{05} from the LOOCV procedure is similar to the XCD_{05} calculated from the measured ecoregional data set. The root mean squared error (RMSE) and coefficient of variation were calculated using the 24 SEs from the LOOCV procedure and compared to the RMSE and coefficient of variation of the B-C model. The validity of the regression model is summarized by the validation RMSE and its coefficient of variation. A small difference between the validation RMSE and the B-C model’s RMSE indicates a good model. A small coefficient of variation indicates little variation in the SEs.

3. Results

The 25th centile values for the 24 data sets ranged from 22 $\mu\text{S}/\text{cm}$ in the Blue Ridge Ecoregion 66 in North Carolina to 626 $\mu\text{S}/\text{cm}$ in Interior River Valley and Hills of Ecoregion 72 in Illinois (Table 1). The lower 30% XCDs for the 24 data sets are shown in Fig. 3 to more clearly show the region of the XCD containing the XCD_{05} . The upper portions of the XCDs contain values that could not be reliably measured with the available data set.

As the background SC increases, the XCDs for the ecoregions plot further to the right with higher SC (Fig. 3). Similarly, the XCD_{05} identified from the intercept of each XCD with the 5th centile line increases as background SC increases. The genera that contribute most directly to each XCD_{05} are the most salt-intolerant genera in each ecoregion. XCD_{05} values ranged from 69 to 1127 $\mu\text{S}/\text{cm}$.

Having derived XCD_{05} values and estimates of measured background SC for 24 data sets (Table 1), the log10-transformed XCD_{05} values were regressed against log10-transformed background SC values to generate a predictive model (Fig. 4).

The regression model using the estimated background SCs from the 24 state data sets is a strong model (Pearson’s $r = 0.93$) (Fig. 4). The B-C model is described by Eq. (1):

$$Y = 0.658 X + 1.071 \quad (1)$$

Where:

X is the log10 of the ecoregion background SC ($\mu\text{S}/\text{cm}$).

Y is the log10 of the predicted XCD_{05} ($\mu\text{S}/\text{cm}$).

The lower 50% prediction limit (PL) from the mean regression line can be calculated to identify when there is a 75% probability that an XCD₀₅ derived by the field XCD method for a new ecoregion would be equal to or greater than the y-coordinate of the lower prediction limit. The 50% PLs were used when choosing among B-C derived values, XCD derived value, or an intermediate value for a SC criterion (Cormier et al., 2018a).

The upper and lower PL for a predicted log₁₀ XCD₀₅ value can be calculated from the regression line using Eq. (2) (Zaiontz, 2014) and log₁₀ transformed SC values (x) as follows:

$$\hat{y} \pm t_{\alpha/2, n-2} S_y \sqrt{1 + \frac{1}{n} + \frac{(x_0 - \bar{x})^2}{SS}} = PL \quad (2)$$

Symbol	Explanation	Example from the B-C model
$\hat{y}$	Log ₁₀ of mean predicted XCD ₀₅ from Eq. 2	Calculated from Eq. 2
N	Number of samples in the model	$n = 24$
α	Alpha error rate for prediction interval (desired confidence level)	50% prediction interval ($\alpha = 0.5$)
t_{n-2}	t-value at specific level (alpha, α) and degrees of freedom ($n - 2$) of interval	For 50% prediction interval ($\alpha = 0.5$), $t_{(1-0.5)/2, 24-2} = 0.686$
S_y	Residual standard error of prediction (standard deviation)	$S_y = 0.11$
SS	Sum of square of x deviation from their mean, $SS = \sum_{i=1}^n (x_i - \bar{x})^2$	$SS = 4.22$
$\bar{x}$	Mean of x values used in the B-C model generation	$\bar{x} = 2.15$
x_0	x value for a new prediction interval	Log ₁₀ background $\mu\text{S/cm}$
PL	Upper and lower prediction limits of mean predicted $\hat{y}$	

The results of validation of the B-C Model that used a LOOCV procedure are shown in Fig. 5. The log₁₀ RMSE for the cross validated model is 0.118 $\mu\text{S/cm}$, which is a corrected measure of prediction error, averaged across all 24 regions, and its coefficient of variation is 0.048. The log₁₀ RMSE for the B-C model derived from the XCD₀₅ values of the observed 24 XCDs is 0.108 $\mu\text{S/cm}$, and its coefficient of variation is 0.044. Both RMSEs and their coefficient of variations are small and the small difference between the LOOCV RMSE and the B-C model RMSE indicates that the model is supported by this validation exercise.

4. Discussion

Many countries generate water quality guidelines to protect aquatic life. Most rely upon laboratory test data to derive aquatic life criteria (e.g. Stephan et al., 1985; CCME, 2007; European Commission, 2011; Warne et al., 2015). A few countries have methods for using other forms of data such as microcosm and mesocosm data (CCME, 2007; van Vlaardingen and Verbruggen, 2007; European Commission, 2011; Warne et al., 2015). However, methods for developing aquatic life criteria using field observational data are not formally defined or recommended for toxicants although they are used for nutrient criteria (U.S. EPA, 2000) and for pathogens in recreational waters (U.S. EPA, 2012). In the United States, there is only one

approved field-based method for developing water quality benchmarks for SC (U.S. EPA, 2011, 2016). The only application of the U.S. EPA field-based method has been for SC. The field-based method was developed because laboratory-based methods did not represent the most salt-intolerant genera and did not measure the relevant ecological effects (U.S. EPA, 2011; Cormier and Suter II, 2013; Clements and Kotalik, 2016). Extirpation of benthic invertebrates occurs at low levels of SC with similar ionic mixtures (e.g. Merriam et al., 2011; Gerritsen et al., 2010; Palmer et al., 2010; Lindberg et al., 2011; U.S. EPA, 2011; Bernhardt et al., 2012; Cormier et al., 2013; Timpano et al., 2015; Dunlop et al., 2015; Zhao et al., 2016). The modes of action that likely lead to extirpation in the field have also been studied in mesocosms and have corroborated effects observed in the field (Clements and Kotalik, 2016). Also, recent toxicity studies have begun to bridge the gap between physiological studies and field observations (Kefford et al., 2004; Kunz et al., 2013; Wang et al., 2016, 2017; Erickson et al., 2017; Mount et al., 2016).

A technical impediment of the field-based method is the need for very large data sets of paired biological and chemical observations. The B-C model resolves this technical challenge by describing the relationship between background SC and 5% extirpation of benthic invertebrate genera. With this B-C model, it is possible to calculate an aquatic life criterion using background SC for a stream as the independent variable. This enables the development of field-based SC aquatic life criteria with sparse data. Furthermore, it accommodates the natural variability of background SC.

This technical advance was possible because there was sufficient data to develop the B-C model and to confirm that the most salt-intolerant genera have XC_{95} values greater than background conductivity. Genera occurred in the lowest SC in each of the 24 study areas and the lowest XC_{95} values within each region were relative to the background SC for each study area (Fig. 3). Thus, sets of benthic invertebrates from similar background SC had similar XCD_{05} values (Fig. 4). This indicates that although a taxon may differ from region to region, there are species with low SC tolerances that occupy the lowest SC waters in a region. That supports the expectation that comparable XCDs are representative of similarly exposed aquatic communities.

When the background SC and XCD_{05} value for each region are log scaled, background SC is linearly related to the XCD_{05} . The B-C regression model of that relationship was validated using a LOOCV procedure which showed that the predictive performance of the model was strong. This regular and biologically relevant relationship between background SC and XCD_{05} further supports the inference that the XC_{95} values in the lower portion of the XCDs would be similar in different places with similarly exposed communities even though the represented genera may differ among those places.

This particular regression model was developed using SC data from waters with ionic mixtures dominated by sulfate and bicarbonate anions and where background SC did not exceed 626 $\mu\text{S}/\text{cm}$. Therefore, the model is only appropriate for waters with these specific ionic characteristics. Furthermore, the individual XCD_{05} values may have limited use as stand-alone values because some XCD_{05} values were calculated using small data sets with an upper SC range that limited the measurement of XC_{95} values. To help select between

using the XCD method and the B-C model, a decision flowchart was developed (Cormier et al., 2018a). Selection of an XCD_{05} from the flowchart involves considering the characteristics of available paired chemical and biological data sets. Confidence in SC XCD_{05} values is based on the size of the data sets, the method for estimating the XCD_{05} values, and ecoregional SC disturbance. The level of ecoregional SC disturbance was judged by comparing the background SC (the 25th centile of the data set used to calculate a XCD_{05}) and an estimate of natural base-flow SC modeled from geophysical attributes in the region. Using that decision process, 63 example XCD_{05} values were calculated for Level III Ecoregions in the United States with comments on relative confidence in those estimates (Cormier et al., 2018a).

In some cases, the 25th centile of the data sets used in model building did not represent natural background for > 20% of streams in an ecoregion. If the estimated XCD_{05} is based on an inflated background, then the XCD_{05} would not be protective. Some of these state data sets may represent least disturbed rather than minimally affected background SC (sensu Stoddard et al., 2006). Natural background SC is the range of ionic concentrations naturally occurring in waters that have not been influenced by human activity. Minimally affected background is an estimate of natural background defined as the background SC in the absence of significant human disturbance. Least disturbed background refers to the background SC given the present state of the landscape. Therefore, a weight-of-evidence approach was developed to distinguish whether a calculated background SC represents minimally affected or least disturbed conditions (Cormier et al., 2018b).

The interpretation and use of the XCD_{05} is influenced by the degree of deviation from natural background. The mean natural base-flow background SC can be estimated from an empirical geophysical model (Olson and Hawkins, 2012). Typically, the predicted geophysical means are greater than the 25th centile of the data sets from a mixture of sites that are neither a probabilistic data set nor composed of only reference sites. However, if the 25th centile SC estimate of background for the data set is greater than the predicted mean base flow SC for reference condition; then, the 25th centile SC may represent least disturbed background (i.e. background for regions with extensive disturbance such as irrigated agriculture). Because the 25th centile may represent a contaminated condition, the biota may already be affected by high SC in those ecoregions. In these places, the derived XCD_{05} represents the level that may extirpate 5% of remaining taxa and may not be protective of the native biota that were common in the past. For example, the predicted mean base flow SC was calculated from geology and other natural parameters of the Central Corn Belt Plains (Olson and Hawkins, 2012). The predicted natural mean base-flow SC (267 $\mu\text{S}/\text{cm}$) was 42% lower than the 25th centile from an U.S. EPA survey data set that measures present day conditions (465 $\mu\text{S}/\text{cm}$). It is likely that the measured background of 465 $\mu\text{S}/\text{cm}$ represents the least disturbed rather than minimally affected conditions in this region. For such areas with extensive modification of background SC, provisions might be considered for exceptional waters in that ecoregion where the SC regime may more closely resemble minimally affected.

5. Conclusions

Evolution and natural selection have resulted in species that occupy low conductivity niches in fresh water (Cormier et al., 2013, Kefford et al., 2016; Olson and Hawkins, 2017). This relationship between the lowest SC habitats and occurrence of the least-salt tolerant species can be used to predict extirpation of aquatic invertebrates as the concentrations of dissolved salts increases. The model presented here will allow others to estimate with varying certainty the change in SC that is likely to extirpate 5% of benthic invertebrate genera in a stream.

6. Data sets

Data sets and individual XCD results used to develop the B-C model are available at the U.S. EPA Environmental Dataset Gateway ((<https://doi.org/10.23719/1371707>) (Cormier, 2017). Data are contained in three zip files. The folder “Biological.zip” contains occurrences of benthic invertebrate genera in 24 state data sets. The folder “Environmental.zip” contains environmental data sorted into 24 data sets. The folder “model.zip” contains the calculated XC_{95} values, probability of observation plots as generalized additive models, and the cumulative frequency distribution for benthic invertebrate genera from the 24 data sets used to develop the B-C model.

A spread sheet for calculating XC_{95} values and XCD_{05} are described in Cormier et al. (2017). The tools, data sets, example calculations, and example outputs are available online at <https://wiley.figshare.com/ieam> and <https://github.com/smcormier/Biological-Extirpation-Analysis-Tools-BEAT/releases/tag/v.1.0.2>. Alternatively, calculation of XC_{95} , GAM plots, XCD_{05} can be calculated using batch R code. The R code and data sets are available on GitHub (<https://github.com/leppott/XC95>). Similarly, the R-code and data sets are available on GitHub (<https://github.com/leppott/XC95>).

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Abbreviations:

B-C background-to-criterion

CFD	cumulative frequency distribution
CV	coefficient of variation
DEC	Department of Environmental Conservation
DEM	Department of Environmental Management
DENR	Department of Environment and Natural Resources
DEP	Department of Environmental Protection
DEQ	Department of Environmental Quality
DNR	Department of Natural Resources
EPA	Environmental Protection Agency
HC₀₅	Hazardous Concentration at the 5th centile of XC ₉₅ values
LOOCV	leave-one-out cross-validation
PCA	Pollution Control Agency
PL	Prediction Limit
RMSE	root mean squared error
SC	specific conductivity
SE	squared error
U.S. EPA	U.S. Environmental Protection Agency
XC	extirpation concentration
XC₉₅	Extirpation concentration values at the 95th centile
XCD	extirpation concentration distribution
XCD₀₅	5th centile of taxa's XC ₉₅ values.

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HIGHLIGHTS

- Salinization of fresh water is inexpensively measured as specific conductivity (SC).
- Loss of taxa are predictable using a model and an estimate of background SC.
- The model can be used to identify protective SC thresholds.
- The method is applicable anywhere with an estimate of background SC.

Fig. 1.

Process for developing the background-to-criterion regression model. CFD = cumulative frequency distribution; SC = specific conductivity; XC₉₅ = Extirpation concentration values at the 95th centile; XCD = extirpation concentration distribution; XCD₀₅ = 5th centile of the distribution of XC₉₅ values. Modified from U.S. EPA (2016).

Fig. 2.

Process for validating background-to-criterion least squares regression model. Left 2 branches depict LOOCV procedure. Right branch describes the characterization of the B-C regression model. B-C = background-to-criterion; CV = coefficient of variation; LOOCV = leave-one-out cross-validation; RMSE = root mean squared error; SC = specific conductivity; SE = squared error; XCD₀₅ = 5th centile of the distribution of XC₉₅ values. Modified from U.S. EPA (2016).

Fig. 3.

The lower 30% of the 24 XCDs. XCD_{05} is the specific conductivity at the 5th centile (horizontal dashed line) of each XCD. The ecoregion legends are ordered from lowest (NC66) to highest (IL72) XCD_{05} . Untransformed SC values are shown on log10 scaled x -axis. The tested range exceeded 1000 $\mu\text{S}/\text{cm}$ for all data sets. SC = specific conductivity; XCD = extirpation concentration distribution; XCD_{05} = 5th centile of the distribution of XC_{95} values. Modified from U.S. EPA (2016).

Fig. 4.

Background-to-criterion empirical model. The log10 scaled x-axis shows the untransformed background specific conductivity estimated at the 25th centile for 24 state data sets. The log10 scaled y-axis shows the XCD₀₅ of XCD shown in Fig. 3. Solid line is the log10-log10 linear regression line. Dotted lines demarcate the 50% prediction intervals, i.e. the probability that a new XCD₀₅ would plot within those bounds is 0.5 and only 25% are expected to fall below the lower prediction limit (lower dashed line). Pearson's correlation coefficient ($r = 0.93$). Data are in Table 1. XCD = extirpation concentration distribution; XCD₀₅ = 5th centile of the distribution of XC₉₅ values. Modified from U.S. EPA (2016).

Fig. 5.

Evaluation of the error in the B-C model by comparison to values for 24 LOOCV regression models. A different symbol is used for each data set. The large symbols are the observed background versus XCD_{05} values from 24 data sets in the B-C model, as in Fig. 4. Each corresponding small symbol represents the LOOCV estimated XCD_{05} value for a particular data set estimated from a model comprised of XCD_{05} values from the other 23 data sets. B-C = background-to-criterion; LOOCV = leave-one-out cross-validation; XCD_{05} = 5th centile of the distribution of XC_{95} values ($XCD_{05} = HC_{05}$). Modified from U.S. EPA (2016).

Table 1.

Paired biological and SC data used to produce the background-to-criterion (B-C) model.

Level III ecoregion	Name	Source of data set	Number of samples ^b	Number of sites	Number of genera	Proportion of unambiguous XC ₉₅ values	25th centile SC, state data sets (µS/cm)	B-C XCD ₀₅ ^b (µS/cm) for model
15	Northern Rockies	Idaho DEQ	614	289	120	0.25	29	142
16	Idaho Batholith	Idaho DEQ	1040	550	136	0.21	42	185
17	Middle Rockies	Idaho DEQ	510	306	110	0.10	136	264
19	Wasatch and Uinta Mountains	Utah DEQ	773	152	69	0.20	271	299
23	Arizona/New Mexico Mountains	Arizona DEQ	374	106	97	0.16	191	249
45	Piedmont	North Carolina DENR	665	433	212	0.26	68	138
47	Western Corn Belt Plains	Minnesota PCA	473	404	106	0.11	587	934
50	Northern Lakes and Forests	Minnesota PCA	734	596	176	0.13	108	320
51	North Central Hardwood Forests	Minnesota PCA	583	437	147	0.22	325	494
52	Driftless Area	Minnesota PCA	344	277	83	0.12	534	655
54	Central Corn Belt Plains	Illinois EPA	469	337	122	0.46	626	813
58	Northeastern Highlands	New York State DEC	383	383	72	0.10	50	212
59	Northeastern Coastal Zone	New York State DEC	277	277	42	0.14	350	706
60	Northern Allegheny Plateau	New York State DEC	562	562	72	0.12	132	248
64	Northern Piedmont	Maryland DNR	710	584	105	0.48	150	227
65-N	Southeastern Plains	Maryland DNR	501	400	92	0.57	99	243
65-S	Southeastern Plains	Mississippi DEP	457	361	127	0.27	38	131
66	Blue Ridge	North Carolina DENR	322	224	176	0.35	22	69
67	Ridge and Valley	West Virginia DEP	926	752	123	0.18	59	154
69	Central Appalachians	West Virginia DEP	1661	1420	142	0.27	94	305
70	Western Allegheny Plateau	West Virginia DEP	2075	1695	139	0.37	169	338
71	Interior Plateau	Indiana DEM	336	290	69	0.23	296	479
72	Interior River Valleys and Hills	Illinois EPA	463	340	116	0.09	462	1127
83	Eastern Great Lakes Lowlands	New York State DEC	591	591	68	0.19	272	525

^aB-C = background-to-criterion; DEC = Department of Environmental Conservation; DEM = Department of Environmental Management; DENR = Department of Environment and Natural Resources; DEP = Department of Environmental Protection; DEQ = Department of Environmental Quality; DNR = Department of Natural Resources; EPA = Environmental Protection Agency; PCA = Pollution Control Agency; SC = specific conductivity; XC95 = extirpation concentration at 95th centile; XCD05 = 5th centile of a taxonomic extirpation concentration distribution.

^bThe data requirements of the XCD method using a minimum of 500 paired biological and chemical samples (see Section 2.1 Data Sets) were not met in all ecoregions; therefore, the calculated XCD05 values are not necessarily example criteria but are reliable enough for development of the B-C model based on the predictive performance of the model. Data sets available at <https://doi.org/10.23719/1371707>.

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