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Understanding ecological impacts in rivers in England and Wales and identifying their possible causes: part 2, The GIS-based Weights of Evidence/Weighted Logistic Regression method

Science Report – SC030189/SR6

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Steve Killeen

Steve Killeen

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Executive summary

An eco-epidemiological approach has been applied to existing biological and surface water chemistry data for England and Wales to investigate its potential in helping identify biological impacts from multiple pressures and understand their causes. The method uses a geographic information system (GIS)-based weights-of-evidence (WOE) and weighted logistic regression (WLR) application for watershed assessment proposed by Kapo and Burton (2006). The spatial association between stressor variables and biological condition is determined by statistically combining stressor concentration maps to predict the locations of known biologically impaired sample sites. Output from the method includes probability maps delineating locations within the study area having the greatest predicted risk of biological impairment, as well as estimates of stressor influence and risk values for the entire study area. The primary objective of this project was to conduct a pilot study to test the applicability of the WOE/WLR method to river data for England and Wales collected by the Environment Agency. As a result, the scope and content of the work in this study was limited by both practical time constraints and data availability.

In this pilot study, ten variables including water chemistry, nutrients, and toxicity (metals and pesticides) were analysed for their spatial association with macrofauna impairment. In this study impairment was defined as sample sites within the 25th percentile of observed:expected macrofauna values based on an Environment Agency reference model. Models for the entire study area were created for the spring season (March-May) and the autumn season (September-November). Additionally, land-use specific models for urban and agricultural land use were created for each season.

The application of the WOE/WLR method to the data was successful. On average, the models successfully predicted 85 per cent of the biologically impaired sites based on the spatial distribution of various stressor concentrations, and accurately predicted 80 per cent of non-impaired sites. Most (86 per cent) of the false positives produced by the model had some degree of impairment present (fewer observed macrofauna than expected).

The spring season model for the overall study area was most influenced by the chloride variable, which may serve as a proxy for stress associated with surface run-off. Biological oxygen demand (BOD) was the most influential variable in the autumn season model for the overall study area, likely representing increases in eutrophication as a result of the seasonal influx of organic matter (leaf fall) combined with existing anthropogenic sources of eutrophication. Ammonia was the most influential variable in the agricultural land use models for both seasons. A poor performance of the pesticide toxicity variable may indicate the need for further refinement of the variable. pH and BOD were important factors in the urban land use model in both seasons. Metals toxicity was most significant in urban land use, particularly during the autumn season. Nitrate, likely from run-off after crop harvest, was a significant factor in the autumn season for both agricultural and urban land use.

Stressor identification and influence information from the WOE/WLR models for the study area were compared to results obtained by a different method, the Effects and Probable Cause methodology (Environment Agency, 2008), which employs a completely different analysis framework, statistical technique, and communicative output. The methods strongly agreed in site stressor identifications (75-80 per cent agreement), however the agreement in the influence of identified stressors at sites (ranked importance) was much lower, though still significant. Differences in model design likely account for differences in the results, with the EPC method utilising raw

species abundance data to attribute stressor influence and the WOE/WLR method directly modelling discrete species loss. A potential option to reduce uncertainty in stressor prioritisation for watershed management is the use of the methods in combination as screening-level lines of evidence, highlighting the importance of stressors identified by both models as significant at a site.

Results from this study yielded macrofauna impairment predictions (location and stressors) potentially useful to river basin managers, and suggest the potential for the WOE/WLR method as a tool for the Water Framework Directive (WFD).

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Tables and Figures

1 Introduction

It remains challenging for watershed managers to effectively prioritise stressors and develop targeted management strategies over large geographic areas. The use of existing monitoring programmes and their data in the development of future watershed management plans is beneficial in terms of cost, time, and effort. The term “eco-epidemiology” in the context of this study refers to the analysis of biological and chemical data in order to identify relationships between biological condition and environmental variables, identify possible or likely causes of stress to the ecosystem, and quantify the effects. Eco-epidemiological approaches range from simplistic to highly complex data analyses, and statistical analysis and modelling can range from having a high degree to almost no input or oversight by the researcher performing the computations. A goal in these studies is to find a compromise between employing statistical approaches that can handle complex ecological relationships, while also allowing for some degree of “expert judgement” in the process to ensure that data relationships are biologically plausible, and not simply data-crunching exercises.

A geographic information system (GIS)-based statistical method combining the techniques of weights-of-evidence (WOE) and weighted logistic regression (WLR) was introduced as an eco-epidemiological tool in a large-scale watershed risk assessment case study in the United States (Kapo and Burton, 2006). The GIS-based WOE/WLR method is a spatial analysis technique that involves combining map patterns of different variables to predict the map pattern of an event of interest. The method was developed as a mineral exploration model in which various regional geologic map patterns were combined to predict undiscovered gold deposits using known regional gold deposit locations as a training dataset (Agterberg *et al*., 1992). In the eco-epidemiological application of the method, spatial patterns of environmental variables are combined to predict the spatial patterns of biologically impaired sites.

In this pilot study, a GIS WOE/WLR analysis was applied to monitoring and spatial data to develop quantitative risk assessment models for macroinvertebrates in catchments of England and Wales. The goal of the study was to test the applicability of the method to the available data, to map the probability of macroinvertebrate impairment across the study area, to generate hypotheses of stressor influence across the study region, and to examine the influence of broad classes of land use on risk assessment hypotheses. Additionally, the results of the analyses were compared with results from an alternate eco-epidemiological technique (Effects and Probable Cause method, Environment Agency, 2008) using the same data sources.

2 Methodology

2.1 Data sources and software

Data sources used in this study included:

- Water chemistry data (hardness, chloride, total suspended solids, pH, biological oxygen demand (BOD), phosphate, ammonia and nitrate).
- Biological sample data (aquatic macroinvertaberate taxon composition and abundance data recorded at Biological Monitoring Working Party (BMWP) level for over 5,000 sites. The data were collected according to highly standardised protocols over the time period 1993-2004. Sampling locations were sampled every three years in spring and autumn as part of the Environment Agency's General Quality Assessment (GQA) protocol.
- Surface water concentrations of a number of toxicants were available (metals and pesticides). Metals included cadmium, chromium, copper, nickel, zinc and lead. Measured total concentrations were converted to bioavailable fractions and the bioavailable fractions were used to calculate local toxic pressures per compound (Potentially Affected Fractions, PAF) and subsequently multi-substance PAF values at each sampling site. Expressing toxicity as a potentially affected fraction (PAF) is a useful way of generating summary statistics for toxic loadings. The Potential Affected Fraction is defined as the fraction of species that can occur locally that is probably affected at a level higher than the 50 per cent effect level. These values were provided by de Zwart (RIVM). Use of a single, multi-substance PAF value per group of compounds minimises the number of predictors in the assessment and so increases statistical power. For a full discussion on the derivation and use of PAF and multi substance-PAF values, please see de Zwart *et al*. (2008).
- For pesticides, the measured data available was limited and typically restricted to old compounds that are no longer approved. Predicted surface water concentrations for pesticides were therefore derived using the Environment Agency's Prediction of Pesticide In the Environment (POPPIE) tool. POPPIE is a GIS-based catchment scale pesticide model. Predicted annual average concentrations were readily available for individual pesticides in England and Wales and were supplied by the Environment Agency to de Zwart (RIVM). A multi-substance-PAF was calculated for total pesticides (see de Zwart *et al*., 2008 for full details)
- Delineated catchment data (UK Centre for Ecology and Hydrology (CEH) 50 km data).
- Classified land cover data from the Land Cover Map 2000 dataset (CEH).

All GIS tasks were performed in ArcGIS version 9.1, with WOE/WLR analysis performed with Spatial Data Modeller version 3.1.81 (Sawatzky *et al*., 2002). Additional statistical analyses were performed in SAS Statistical Package version 9.0.

2.2 GIS-based Weights-of-Evidence and Weighted Logistic Regression

The GIS-based WOE/WLR method for eco-epidemiology involves three major components: 1) study area and variable definition, 2) WOE analysis, and 3) WLR modelling. The WOE analysis identifies potential stressors by examining the strength of spatial association between individual variables and biologically impaired sites, including the variable concentrations at which the association becomes significant. The information from WOE is used to select and optimise stressor variables to be included in the WLR model. The WLR model combines significant variables to predict the probability of site impairment across the study area. The components of the WOE/WLR method are discussed in detail in the following sections.

2.2.1 Data preparation

The study area extent included catchments in England and Wales with biological and water chemistry sample data (Figure 2.1). The most general catchment classification identifier was used in order to best represent the largest study area scale, while omitting major drainage areas lacking sample data. For a number of areas, no data was available and these areas are shown as unshaded in Figure 2.1.

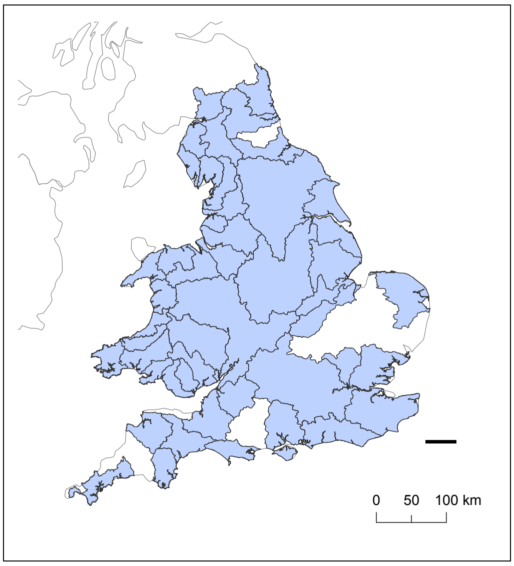

Figure 2.1 Study area extent; catchments containing sample data

Ten water chemistry parameters were examined in this study as potential stressor variables (Table 2.1). Sample data from the time period 1995-2004 was divided into spring (sampling season 1: March-May) and autumn (sampling season 3: September-November) groups for all water chemistry variables with the exception of metals toxicity and pesticide toxicity, which were derived from an external source (De Zwart *et al*., 2008) based on annually grouped data. The mean value for each variable for each site was computed for all ten water chemistry variables. The result was a 10-year averaged spring and autumn season dataset for each variable, with the exception of metals and pesticide toxicity, which had an annual averaged dataset each. A discussion of data variability is provided later in this report (Section 3). GIS raster maps for the study area were created for each variable by interpolating sample point concentrations. The raster maps were created using localised interpolation, where grid cells are assigned the variable value of the nearest sample point at a grid cell resolution of 0.25 km^2. Interpolated estimates for each variable were made only for study area catchments containing sample data. Any study area catchments lacking data for a particular variable had a “null” value in the variable raster map. To reduce noise in the data and prepare the maps for WOE analysis, the raw values of each variable raster map were ranked into five general classes (value ranges) from low to high using Jenk’s Natural Breaks classification algorithm in ArcGIS. Jenk’s Natural Breaks was chosen because it produces a gradient of value classes having minimal variability within each individual class.

Table 2.1 Water chemistry variables

Parameter	Abbreviation (Units)	*N* sites (Spring, Autumn)
Ammonia	NH_4^+ (mg/L, ionized as N)	901, 901
Biological Oxygen Demand	BOD (mg/L, ATU as O2)	901, 901
Chloride	Cl^- (mg/L, chloride ion)	880, 897
Hardness	$CaCO_3$ (mg/L, total CaCO3)	901, 901
Nitrate	NO_3^- (mg/L as N)	900, 901
Orthophosphate	PO_4^- (mg/L as P)	901, 901
pH	pH (standard units)	901, 901
Suspended solids	TSS (mg/L at ˚C)	898, 829
Toxicity, metals	Metals (% species affected, msPAF[1])	294 (annual value)
Toxicity, pesticides	Pest (% species affected, msPAF[1])	350 (annual value)

Notes: [1]msPAF = multi-substance potentially affected fraction of species (Posthuma and De Zwart 2006), data provided by De Zwart *et al*. (2008). This variable represents the percentage of macrofauna species exposed to their EC_{50} for one or more metals and pesticide concentrations at a site.

Biological sample data was used to develop biological training point datasets for the WOE/WLR analysis. The Environment Agency used RPBATCH III+:RIVPACS (River Invertebrate Prediction and Classification System) Release 3.3 to produce the probability of capture (Pc) of each BMWP family and the expected abundance for each family at each site. The Pc values are summarised over species per site by calculating the observed-expected ratio (O/E_{site}). A high O/E indicates a favourable site. RIVPACS O/E values for years within the study time range (1995-2004) were separated into spring and autumn season groups (spring *N* sites = 889, autumn *N* sites = 881), and the mean O/E value per site was determined for each season (average of two samples per site per season). A training dataset definition for impaired biological sites was created by selecting the 25th percentile of all RIVPACS O/E values, which corresponded to a value of O/E ≤ 0.66. A training dataset definition for high-quality biological sites, also required for the WOE/WLR analysis, was created using the highest 25 per cent of O/E values, a threshold value of O/E > 1.00. The end result was an impaired and high-quality training dataset for both spring (impaired *N* sites = 216, high-quality *N* sites = 195) and autumn (impaired *N* sites = 210, high-quality *N* sites = 211), respectively. Sites with O/E> 0.66 but <1.00 were excluded from use as training sites in this study, but were used to evaluate model fit, as described later in the Results section.

2.2.2 Weights of evidence method

The water chemistry variable raster maps and the impaired and high-quality site training point datasets were used in WOE analyses. The WOE analysis is a data exploration exercise to delineate which variables, and which variable values, most significantly increase the odds of the occurrence of a training site. The analysis takes into account the prior odds (chance observation) of a training site given the extent of the study area. Both impaired (O/E < 0.66) and high-quality (O/E > 1.00) sites were independently used as training site datasets in separate WOE analyses, to adjust for sampling bias and detect biologically relevant trends.

Raster cell calculations are used to compute the prior odds of observing a training site (y) over the entire study area (all catchments) independent of other variables, as $\frac{p\{y\}}{p\{\bar{y}\}}$ (simply the proportion of raster cells containing a training site divided by the proportion of raster cells without training site).

Next, the posterior odds of observing a training site both within, $\frac{p\{y \mid x_i\}}{p\{\bar{y} \mid x_i\}}$, and outside, $\frac{p\{y \mid \bar{x}_i\}}{p\{\bar{y} \mid \bar{x}_i\}}$, each of the five Natural Breaks value classes for each of the 10 stressor variables was calculated. The ratio between the prior and posterior odds is referred to as a weight ('W'), and a pair of weights ('W^+' for within and 'W^-' for outside a value class) was computed for each of the five value classes for each of the 10 stressor variables. The difference between the weight pairs, 'W^+ - W^-', called the 'contrast' value, is computed for each value class as an overall measure of spatial association between the value class and the training sites. A contrast value of zero is equivalent to association by random chance, a positive contrast indicates a positive association between site occurrence and the value class, and a negative contrast indicates a negative association between site occurrence and the value class. An adjusted 'studentised' contrast value is used to interpret significance, with a studentised contrast confidence value of +/- 1.95 approximate to 95 per cent confidence (Robinson and Kapo, 2004).

Figure 2.2 shows a plot of the computed studentised contrast values for the raster map for BOD (spring season), showing the odds of impaired and high-quality site occurrence over the five-class concentration gradient of the variable. A similar plot is produced for each variable. In the example for BOD (spring season) in Figure 2.2, impaired sites are much more likely to occur above a value range of 2.98-4.09 mg/L, while high-quality sites are generally more likely to occur below this value range.

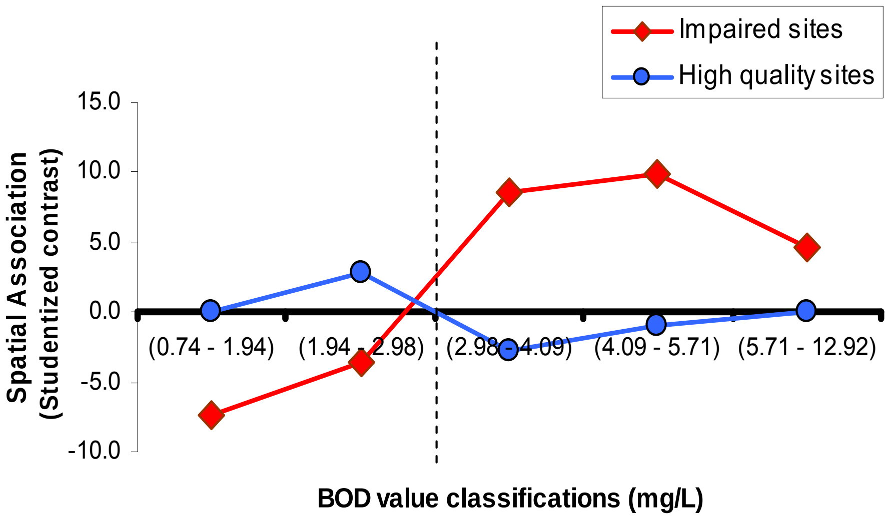

Figure 2.2   Example Weights-of-Evidence analysis plot for BOD (spring).

The plotted WOE trends are used in an expert judgement process to evaluate whether a water chemistry variable was a potential stressor, based on evidence of a positive association with impaired sites combined with an inverse or unrelated trend for high-quality sites. Variables that did not show any response over the gradient, or whose response was similar between impaired and high-quality sites, were dropped from further evaluation. The threshold value range, shown as a dotted line in Figure 2.2, is the point at which association with impairment became positive for the variable. In the BOD example presented in Figure 2.2, this range is 2.98-4.09 mg/L). This was used to simplify the raster maps for each identified potential stressor into a binary map, with a value of "1" attributed to stressor values having increased odds of impairment (for example in the BOD example, >2.98 mg/L), and a value of "0" given to values having decreased odds of impairment (BOD ≤ 2.98). The rationale for this step is to improve the weighted logistic regression model by optimising the individual input variables for maximum predictive strength (Robinson and Kapo, 2004). Relationships need not be linear- non-linear relationships; for example stress associations at low and high values of a stressor can be addressed by grouping all values associated with stress together (binary =1), or creating separate variables to represent the different types of response. In this study, however, no stressor variables examined had a strong enough trend of this type to be delineated at the large scale of the study area and general biological endpoint evaluated.

A new set of WOE analyses were run for the binary stressor variables, yielding a single contrast value for each variable. Stressor variables having a contrast value with $p< 0.1$ confidence were selected for input into the weighted logistic regression model. The stressor variables selected for the various models in this study are listed later in the Results section (Tables 3.1, 3.2, and 3.3).

2.2.3 Weighted logistic regression

Weighted logistic regression (WLR) was used to integrate the new binary raster maps delineated in the WOE analysis for each potential stressor to predict the locations of impaired sites over the entire study area extent. WLR models the probability of impairment as a function of the unique combinations of stressor variables. Before final model convergence by maximum likelihood estimation, the unique combinations are weighted by the amount of map area they occupy to adjust for the fact that large areas are more likely to contain a site based on random chance. Further information on WLR can be found in Agterberg (1992). WLR does not assume variables are independent, allowing for collinearity among variables without impacting model predictions (Robinson and Kapo, 2004). However, due to the effects of multicollinearity on confidence of interpretation of the parameter coefficients, collinearity diagnostics were performed using SAS Statistical Package. Variance inflation factors (VIF) were computed on both the raw and binary values of the stressor variables inputted into the WLR models to determine the amount of error associated with the parameter coefficient due to collinearity. The most conservative VIF threshold of >2.5 was selected as a value of potential concern. If a stressor variable had a VIF value of >2.5 but had a significant WLR coefficient ($p<0.5$), the interpretation of the coefficient was sound, but if the WLR coefficient was not significant, the stressor variable was removed from the WLR model. This process ensured that the magnitude of the WLR coefficients (that is, stressor influence) could be compared between stressor variables with confidence.

The results from a WLR model include an impairment probability map for the study area, and a ranking of the relative influence of the individual variables (WLR coefficients). The WLR coefficient indicates the increase in odds of impairment when moving from a binary value of 0 to 1. Separate WLR models were created for spring and autumn seasons for the study area. Model fit for WLR was determined by overlaying all UK RIVPACS sample points for a season over the impairment probability model map and computing the proportion of sample values correctly predicted by the model, as well as false positives and false negatives. A correct prediction would be a RIVPACS O/E value ≤ 0.66 in WLR map areas with elevated impairment probability (above the mean WLR model value), or a O/E value > 0.66 in WLR map areas with low impairment probability (mean WLR model value or below).

2.2.4 Evaluation of sample variability

An area of potential concern in this study was the grouping of 10 years of data (1995-2004) into representative seasonal mean values for the various variables. A limitation of the WOE/WLR method is that because geographic maps are used for the statistical analyses, there cannot be more than one representative value per location for a particular model. If various years were to be explored separately, it would require a separate WOE/WLR model for each year, a feasible task but beyond the practical scope of this case study. The use of seasonal groupings sought to reduce variability in the grouped data, as well as allow study of seasonal relationships. To address how much increased variability the use of 10-year seasonal groupings introduced compared to the alternative use of means computed for a group of few years, including looking at one year, a brief examination of sample variability was conducted by comparing the site standard deviations for the 10-year seasonal groupings with data grouped for only three years and only one year. Results from this analysis are presented in Section 3.2.

2.3 Cross-comparison with effects and probable cause methodology

Stressor identification and prediction of the most influential stressors for the study area from the WOE/WLR method were compared with results from an alternate eco-epidemiological method, the Effects and Probable Cause (EPC) approach (de Zwart *et al*., 2006), performed for the same study area and variable types (de Zwart *et al*., 2008). The EPC approach uses Poisson regression to model species abundance as a function of the continuous (raw) distributions, water chemistry variables and natural factors. Species missing from sites are determined using RIVPACS. The species abundance Poisson models for all species missing from a particular site are used to estimate the contribution of each stressor variable to decreased species abundance at a site. This is computed by summing the negative variable coefficients for each model, dividing the individual coefficients by the sum to attain the individual percentage stressor variable influence, and then averaging the percentage influence for each stressor over all models for missing species at a site. The results are visually displayed as pie charts on a map, with pie size related to 1 minus the RIVPACS value (larger size = more impacted), with the pie slices proportional to the site stressor influence. For more information about the EPC model, see de Zwart *et al*. (2006, 2008).

The site predictions as stressor percentage contributions from the EPC model, were computed by year, yielding multiple results for each site. In order to directly cross-compare with the WOE/WLR method, which grouped years together, the mean percentage stressor contribution of each variable was computed for each site over all years (1995-2004), and these results were compared with WOE/WLR results for the spring and autumn season, respectively. Another difference between the methods is the requirement of the EPC method to have co-located data for all variables (each site must have a sample value for all variables, N = 307 sites), while the WOE/WLR method handles data gaps for one or more variables using interpolation or null values, allowing for more sample sites to be included. We were therefore able to include more sites from England and Wales in this study than could be included in the EPC approach.

A subset of WOE/WLR impaired sites that were also used in the EPC model were used to cross-compare stressor identification and influence results (*N* sites spring = 62, *N* sites autumn = 57). Three major cross-comparison exercises were conducted between the methods:

- A comparison of site stressor identification per site.
- A comparison of dominant (most influential) stressors.
- A comparison of the relative influence (ranking) of identified stressors.

A stressor was identified by the WOE/WLR method at a site if the stressor had a binary value of 1. While the EPC method did not have a clear threshold for site stressor identification, for the purpose of this study a stressor identified at a site by the EPC method had an average contribution of at least 1 per cent to the abundance models for missing species at the site. This value was chosen because a discrete threshold needed to be set in order to compare between the WOE/WLR and EPC methods, and the EPC method attributed small amounts <1 per cent of stress contribution to every stressor variable as an artefact of its averaging scheme. A selected threshold of ≥1 per cent stress contribution as an EPC stress identification resulted in a similar number of identified stressors per site between the WOE/WLR and EPC methods (~ 3-4 per site). If a variable at a site met both these criteria (WOE/WLR binary = 1, EPC contribution ≥ 1 per cent), the methods had a “match” in stressor identification. Similarly, if a variable at a site did not meet both these criteria (WOE/WLR binary = 0, EPC contribution < 1 per cent), the methods also had a “match” (the stressor was not identified by either method). The overall “per cent matching” was computed for both the WOE/WLR spring and autumn season cross-comparisons with the EPC method, and the significance of this value was determined using Cohen’s Kappa statistic, which adjusts for agreement due to chance.

A cross-comparison of dominant stressors identified by the methods was conducted by computing the frequency of the highest-ranked site stressor variables, over all sites. In the WOE/WLR method, stressor rankings at a site were determined by the magnitude of the WLR coefficient for identified stressor variables, while in the EPC method variable rankings were determined by the average percentage contribution of identified stressor variables to the species abundance models for the site. To further compare stressor influence between the methods, stressor variables identified by both methods at a site were attributed a rank based on the ranking criteria just discussed, and a correlation analysis was performed between the rank values over all sites. This comparison provided information about how similarly the methods ranked stressor variables in importance.

2.4 Land use specific analyses

Additional WOE/WLR analyses were conducted for spring and autumn season data considering two specific land use types. For the land use specific analyses biological and water chemistry variables were adjusted to include only those occurring within dominant land cover classifications of agricultural and urban land use. Classified data from the Land Cover Map 2000 (LCM2000, CEH) was generalised into an urban category (LCM2000 classes “171” and “172”) and an agricultural category (LCM2000 classes “41”, “42”, and “43”). Impairment probability maps and stressor rankings were created and model fit evaluations were performed for urban and agricultural land use model for each season.

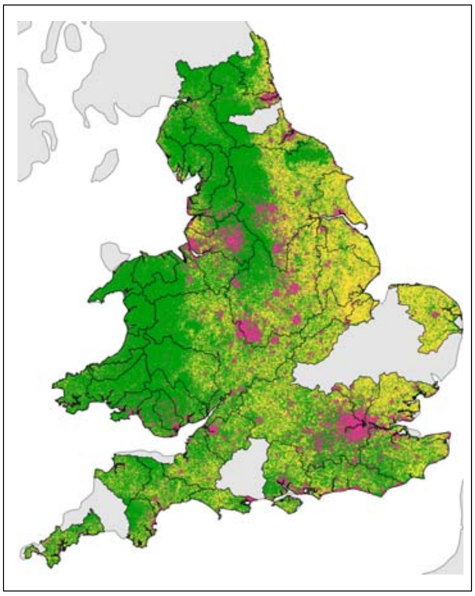

Figure 2.3 General land cover classifications for the WOE/WLR study area (yellow = agriculture, red = urban, green = other) based on LMC2000 data (CEH).

3 Results

3.1 UK study area WOE/WLR analysis

WOE/WLR analyses for spring and autumn seasons were successfully conducted for the study area. The stressor values above or below which biological impairment was more likely to be observed (binary map value = 1, determined by WOE analysis) are given in Table 3.1 for the stressor variables included in the WLR model. These threshold values are given as ranges based on the original Natural Breaks classification of the variables in the WOE analysis. At this level of analysis, the exact point within the value range where the trend occurs cannot be delineated (that is, the most conservative estimate is at the low or high end, depending upon the variable).

The WLR impairment probability model map (Figure 3.1), which statistically combined the binary stressor maps, delineates areas with the highest probability of impairment. The probability values should be interpreted as relative probabilities (that is, favourability) for the study area, not as literal probability values (Robinson and Kapo, 2004). The map colour gradient from grey to red indicates increasing probability categorised by standard deviations, allowing for direct comparisons between model maps (spring season *vs*. autumn season, and so on). Green to red map areas delineate regions of the study area where sites with impaired macrofauna are most likely to occur. Grey colour indicates either no data, below average, or average impairment probability (similar to random chance). Red colour indicates the highest probability for the occurrence of impaired sites.

The WLR coefficients for each variable (Table 3.2) are used to rank the influence of each stressor in the overall study area model, and at the site-specific level based on the stressor values present at the site. Each unique combination of stressor variables in the raster map has been assigned a WLR impairment probability and an associated ranking of stressors. Each grid cell of the raster map belongs to one of the unique combinations, allowing for an interactive query of impairment probability and stressor influence within the GIS interface.

Table 3.1 UK study area impairment association thresholds for stressors

Model	Stressor	Impairment association threshold range[1]
Spring	Chloride	> (33.2 - 68.6) mg/L
	Ammonia	> (0.15 - 0.55) mg/L
	pH	< (7.6 - 7.9)
	Suspended solids	> (9.3 - 19) mg/L
	BOD	> (2.98 - 4.1) mg/L
	Metals	> (1.8 - 3.9) % species affected
Autumn	BOD	> (2.07 - 2.81) mg/L
	Ammonia	> (0.097 - 0.5) mg/L
	pH	< (7.39 - 7.73) mg/L
	Metals	> (1.8 - 3.9) % species toxicity
	Chloride	> (36.3 - 88.06) mg/L
	Nitrate	> (5.88 - 8.63) mg/L

Notes: [1]The impairment association threshold is the value range determined in WOE analysis above or below which the odds of site impairment increase (classified as a binary map value = 1 for the WLR model). Stressors are shown ranked by influence for each land use/season model.

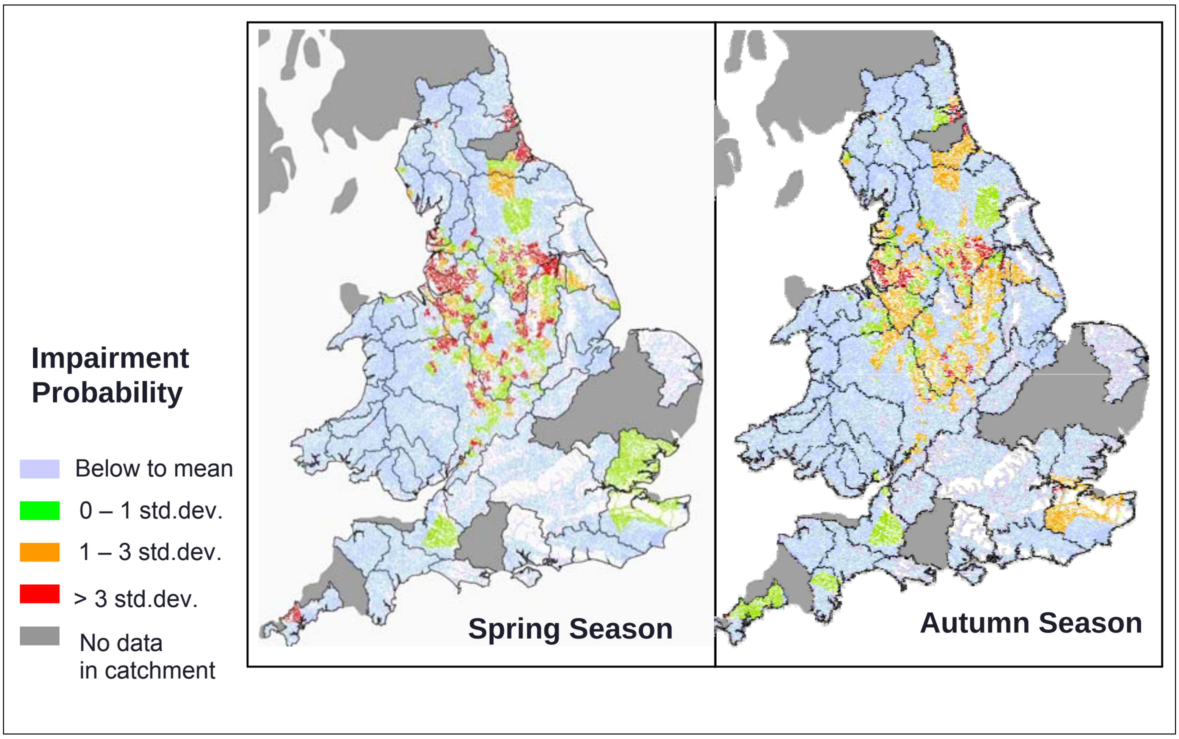

Figure 3.1 WLR impairment probability map for macrofauna, extracted by river network

Chloride and ammonia were the most influential variables in the spring model, while BOD and ammonia were most influential in the autumn model. Suspended solids (TSS) were only significant in the spring model, while nitrate was only significant in the autumn model. The influence of ammonia was consistent between the two seasonal models.

Table 3.2 Ranked stressor variables for the study area (* = Variable had variance inflation factor > 2.5 but a significant WLR coefficient, p<0.05)

Season	Rank	Stressor	WLR Coefficient *(p<0.05 unless noted otherwise)*
Spring	1	Chloride	1.41
	2	Ammonia*	1.35
	3	pH	0.85
	4	Suspended solids	0.40
	5	BOD	0.34
	6	Metals	0.26 (*p* = 0.09)
Autumn	1	BOD	1.47
	2	Ammonia*	1.37
	3	pH	0.64
	4	Metals	0.56
	5	Chloride	0.39
	6	Nitrate	0.26 (*p* = 0.11)

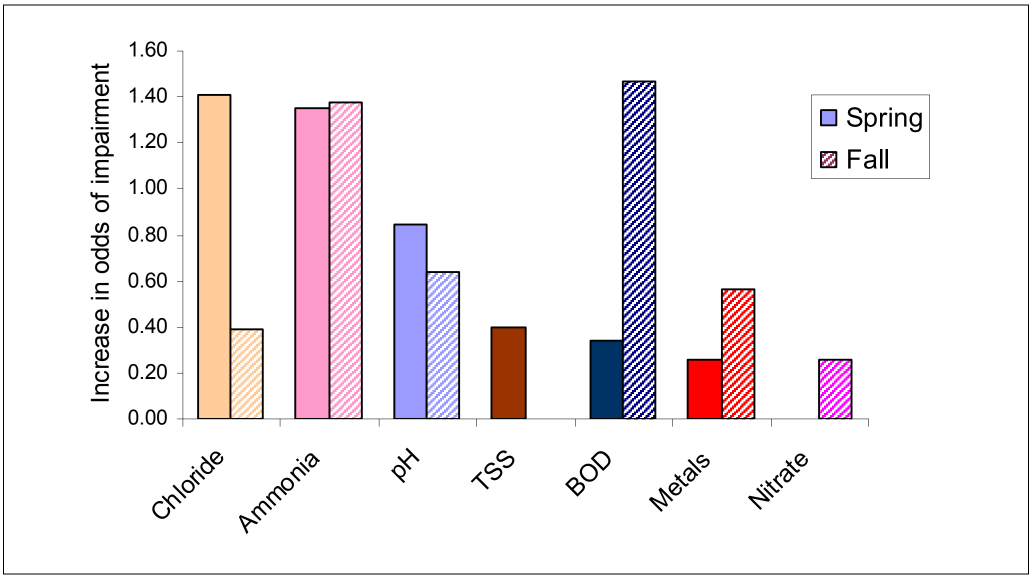

Figure 3.2 Stressor influence (WLR coefficients) for seasonal models

Model fit evaluations were performed for the spring and autumn models. When overlaying all biological sample values (all values of O/E) on the impairment probability map, the overall percentage prediction accuracy (impaired or not impaired) of the models was 75 per cent for spring and 76per cent for autumn, respectively. When evaluating the success of prediction for impaired sites only (O/E ≤ 0.66), the models successfully predicted 81 per cent and 85 per cent of the impaired sites for spring and autumn, respectively. Most of the error associated with the models was due to false positives (the model predicting a site to have O/E ≤ 0.66 when in reality it was higher). Most (56 per cent) of those false positive site predictions for the two models had O/E values of 0.85 or lower. Pearson correlation analyses performed between the site O/E values and the associated predicted impairment probabilities yielded significantly negative relationships for both the spring ($R = -0.59$, $p<0.0001$) and autumn ($R = -0.57$, $p<0.0001$) models. This result indicates that as the probability of impairment increases, the magnitude of impairment (species loss) increases as well (orange and red map areas in Figure 3.1 generally have the worst conditions).

3.2 Sample variability evaluation

The sample variability associated with grouping 10 years of seasonal data compared with an alternative of grouping fewer years of annual data was considered. The frequency distribution of standard deviations associated with the mean site values for each environmental variable were compared between 10-year seasonally grouped data, three-year annually grouped data, and one-year annually grouped data. The variance associated with mean values for 10-year seasonal data did not show a major difference with annually grouped data for three-year or one-year groupings The evaluation of sample variability for ammonia is given in Figure 3.3, suggesting that grouping by season allowed a reduction in variability in the 10-year data comparable to that of grouping of fewer years, and/or the variability in sample measurements at a site acts on a smaller temporal scale than a year.

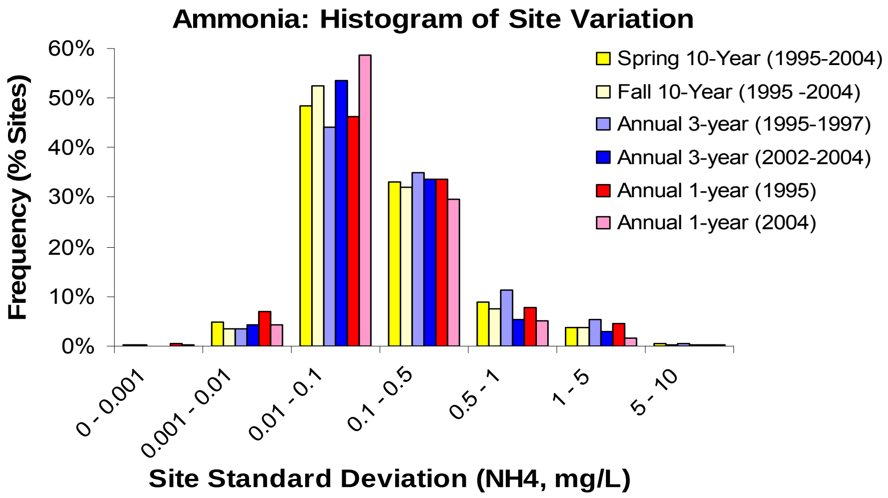

Figure 3.3 Sample variability for ammonia; comparison of year groupings

3.3 Cross-comparison results

The WOE/WLR model outputs were compared with outputs from the de Zwart *et al*. application of the EPC method to the same data set (de Zwart *et al*. (2008)) to see whether the ranked lists of potential stressors identified by each model were comparable. The spring WOE/WLR model and EPC model had a good agreement rate of 80 per cent (Cohen's Kappa = 0.39, $p<0.0001$). On average, the spring WOE/WLR model predicted 70 per cent of the stressors per site predicted by the EPC model, while the EPC model predicted 54 per cent of the stressors per site predicted by the WOE/WLR method. The autumn WOE/WLR model and EPC model had an agreement rate of 75 per cent (Cohen's Kappa = 0.49, $p<0.0001$). On average, the autumn WOE/WLR model predicted 69 per cent of the stressors per site predicted by the EPC model, while the EPC model predicted 72 per cent of the stressors per site predicted by WOE/WLR.

An examination of the dominant stressors, that is, those most frequently ranked the highest at a site, indicated that the dominant stressor in the EPC model was pH, in the spring WOE/WLR model chloride, and in the autumn WOE/WLR model BOD (Figure 3.4).

The methodologies demonstrated little similarity in the way that they ranked stressor variables at a site, despite showing strong similarity in identification of stressors. A Spearman correlation analysis was performed on the site-specific rankings of stressor variables predicted by both the WOE/WLR model and the EPC model. This exercise was performed twice using the spring, and then the autumn WOE/WLR models. As discussed in the methods section, the WLR coefficient magnitude, and the percentage stress contribution were the criteria used to rank site stressors by the WOE/WLR and EPC methods, respectively. The correlation between the site-specific stressor rankings of the spring WOE/WLR model and the EPC model was 0.17 ($p<0.06$). The correlation between the site-specific stressor rankings for the autumn WOE/WLR model and the EPC model was higher and significant at 0.29 ($p = 0.0002$), but still a relatively low value.

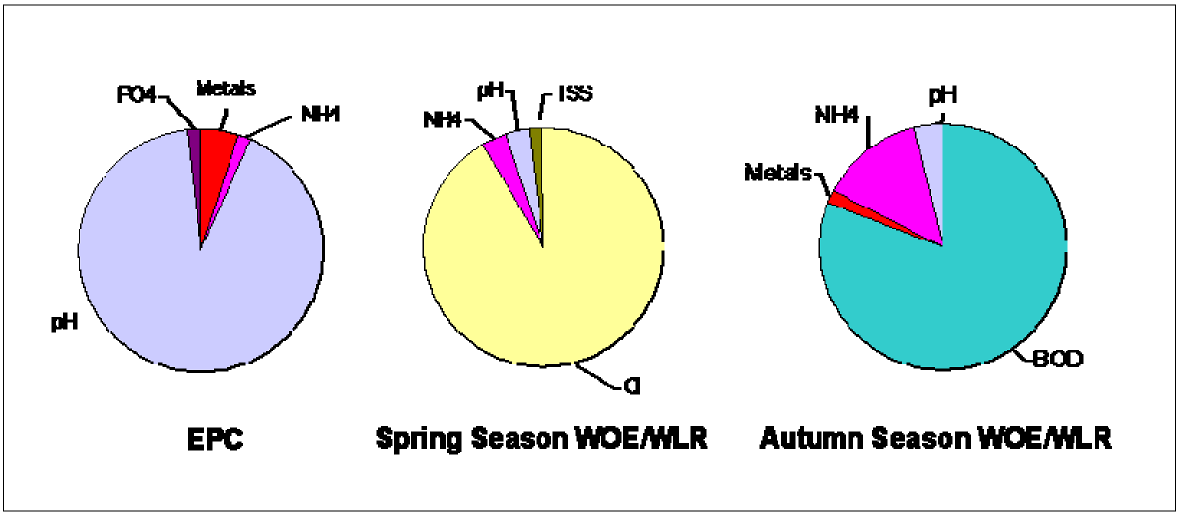

Figure 3.4 Dominant site stressors: frequency of variable as highest ranked (#1) site stressor for EPC and seasonal WOE/WLR models over all sites

The degree of agreement in identification of various stressors between the spring WOE/WLR model and the EPC model, and between the autumn WOE/WLR model and the EPC model, is shown in Figures 3.5 and 3.6, respectively. The most frequent site stressor identification overlap between the spring model and the EPC model included ammonia, BOD, chloride, and pH.

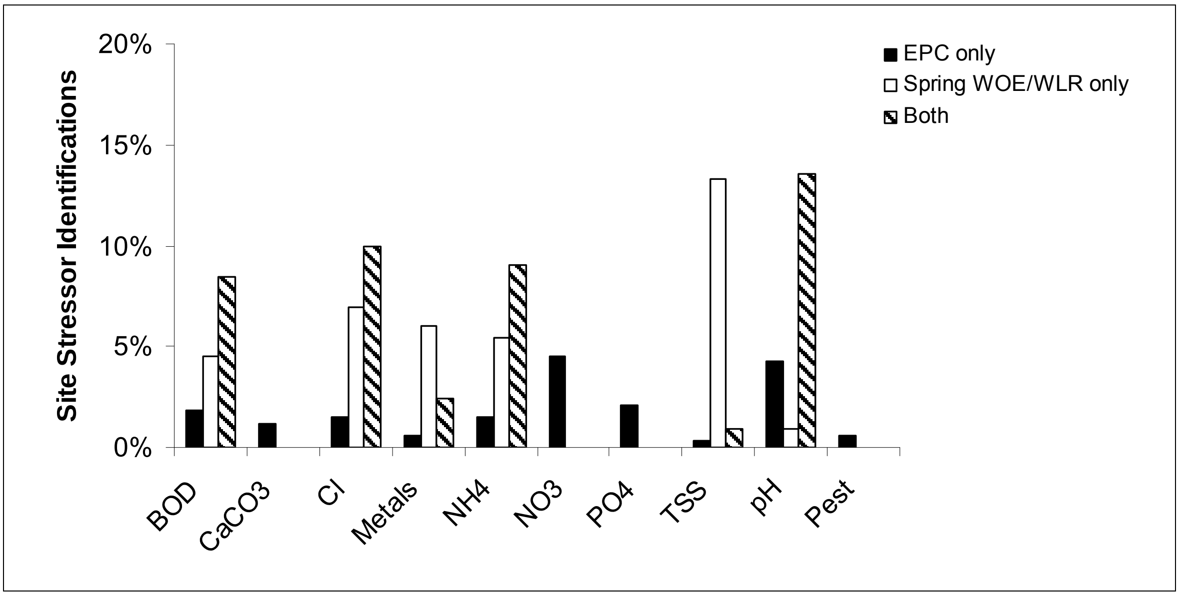

Figure 3.5 Comparison of stressor identification agreement (by stressor) between the spring WOE/WLR model and the EPC model

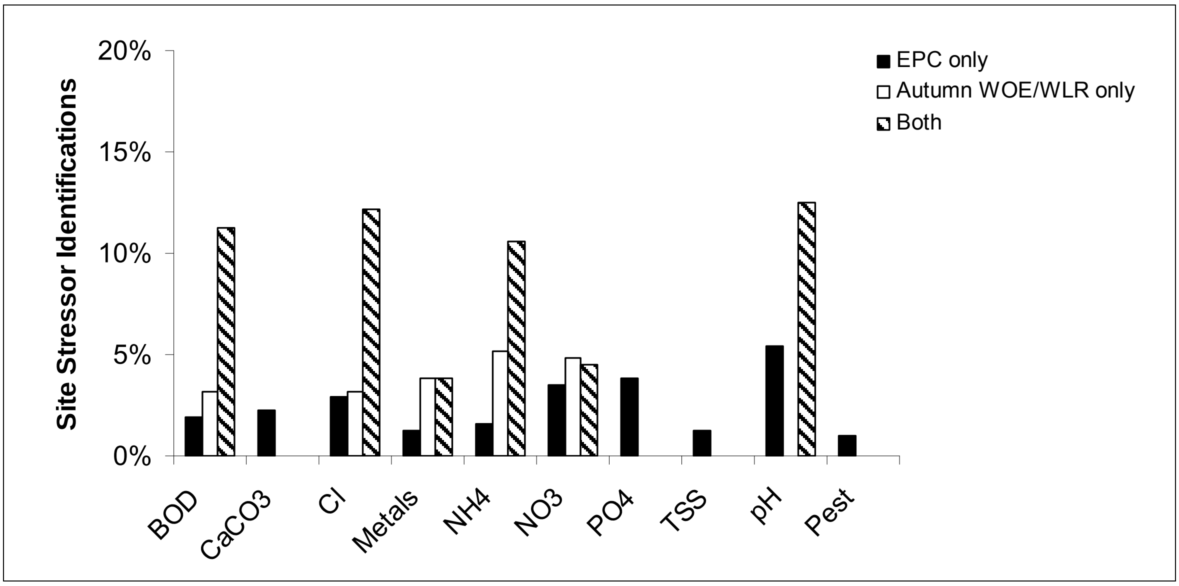

Figure 3.6 Comparison of stressor identification agreement (by stressor) between the autumn WOE/WLR model and the EPC model

3.4 Land use specific WOE/WLR

Impairment probability maps based on land-use specific WLR models for spring and autumn are presented in Figures 3.7 and 3.8, respectively. Visually comparing the models between spring and autumn reveals increased impairment probability (and hence likely severity) in agricultural areas in the northeast of the country, during the spring season. It is surprising that some of the most intensive arable areas in the Anglian region have not been highlighted by this method, but this may be due to missing input data in this area and possibly the nature of the modelled pesticide input data used (see below). In the autumn season, impairment probability is increased in the drainage areas around London, in the NW of England and some locations in central England.

Figure 3.9 shows the relative stressor influence of various water chemistry variables in the land use specific models for both seasons and indicates ammonia is significant in agricultural areas in both spring and autumn. Suspended solids and hardness were exclusively significant stressor variables in the agricultural areas, while pH, phosphate, and metals were more significant in urban areas than agricultural land use. The pesticide toxicity variable was only found to be a significant predictor of impairment in urban land use in the spring season. However, the modelled pesticide data used was unlikely to reflect the peak pesticide concentrations most likely to cause biological effects. Pesticides exposure is peaky and transient in nature, only occurring in certain months of the year for some compounds, depending on use patterns. Annual average modelled pesticide concentrations were used and this will effectively have removed the peak concentrations most likely to cause ecotoxicological effects. For the purposes of this scoping study, the annual average modelled data used was the only data available at a national scale within the timescales of the project. Further work is required to generate more realistic national surface water pesticide concentrations that better represent the typical concentrations that macroinvertebrates are exposed to.

The impairment association threshold value ranges, determined by WOE analysis, for all variables in the WLR model are provided in Table 3.3. These value ranges delineate the variable values above or below which the odds of site impairment increase.

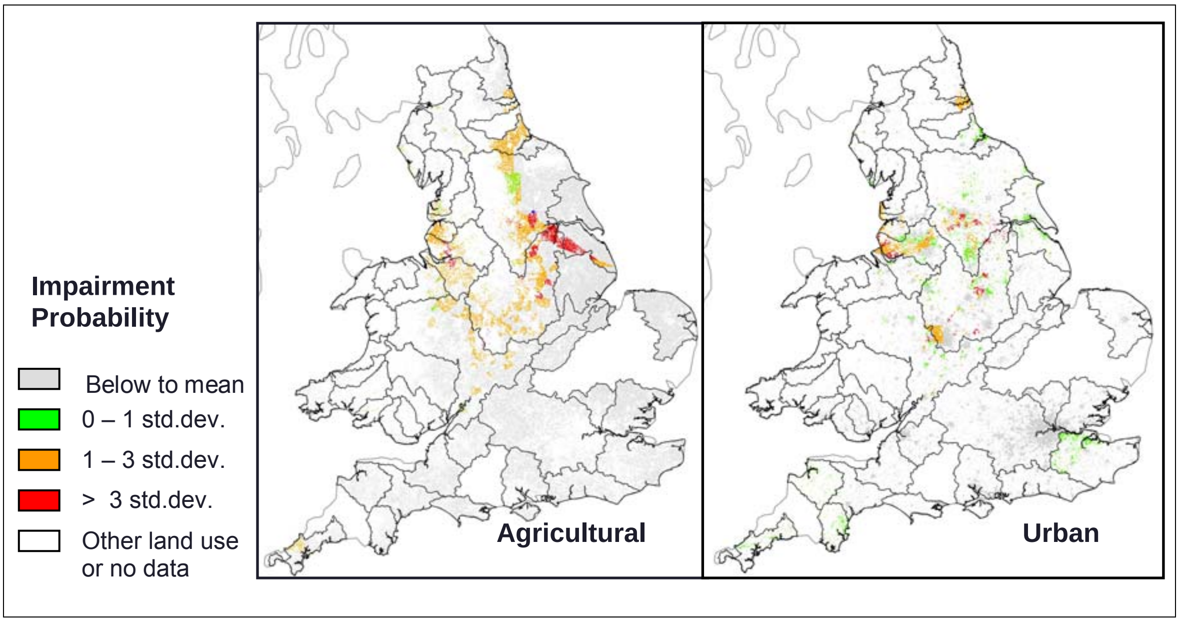

Figure 3.7 Land use specific macrofauna impairment models: Spring season.

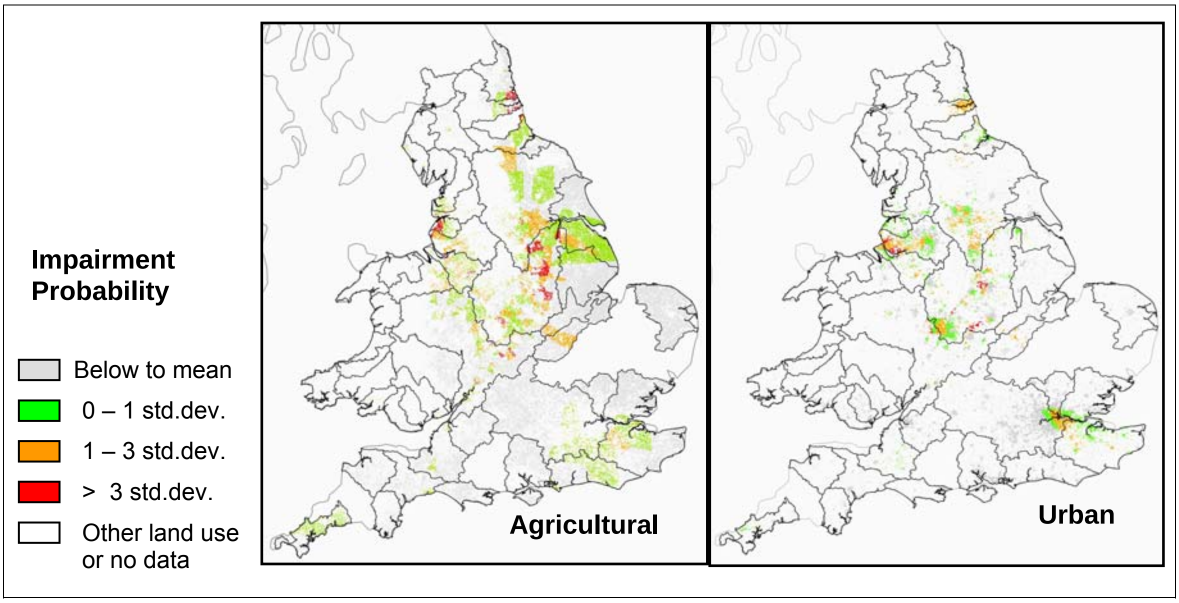

Figure 3.8 Land use specific macrofauna impairment models: Autumn season.

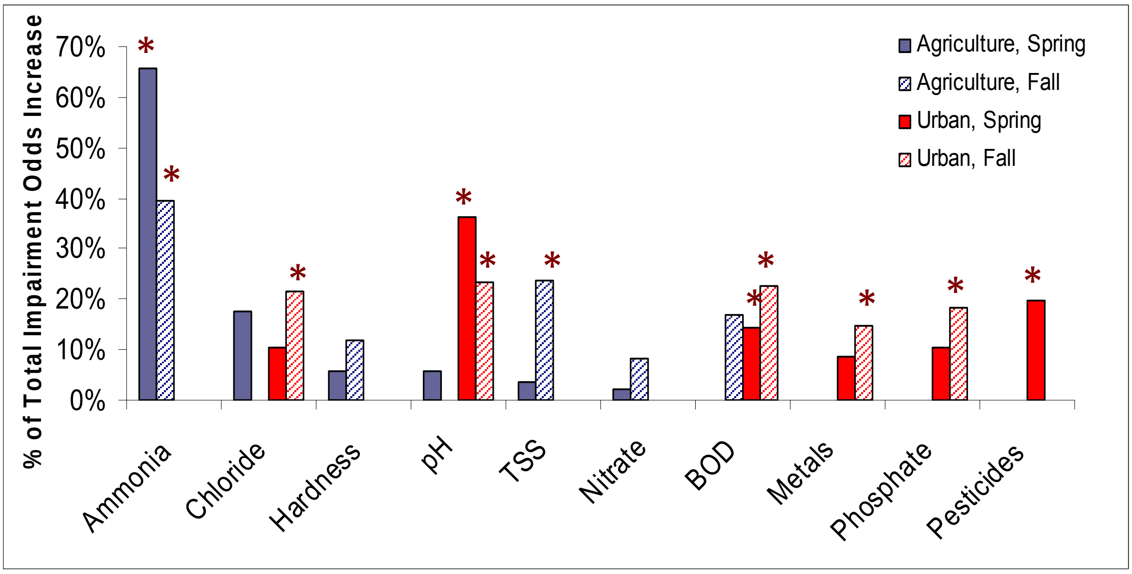

Figure 3.9 Stressor influence (WLR coefficients) for land use specific models. * = WLR coefficient significant at p<0.05.

Model fit analyses for the land use WOE/WLR models found an overall accuracy (comparing predicted biological impairment to actual impairment at all sites) of 85 per cent for the agricultural spring model and 74 per cent for the autumn season model. The overall accuracy for spring and autumn urban land use models was 74 per cent and 72 per cent. When looking at just impaired sites, success rate for prediction of impaired sites (O/E ≤ 0.66) for the agricultural models was 77 per cent for spring and 93 per cent for autumn and for the urban models was 71 per cent for spring and 100 per cent for autumn. As with the overall study area models, observed impairment severity increased as impairment probability increased. Significant Pearson correlations were found between the raw site O/E values and the predicted impairment probability, for both the agricultural models (spring R = 0.56, p<0.0001; Autumn R = 0.5, p<0.0001), and the urban models (spring R = 0.56, p<0.0001; Autumn R = 0.24, p = 0.05).

Table 3.3 Land use specific impairment association thresholds for stressors

Model	Stressor	Impairment association threshold range[1]
Spring, Urban	pH	< (7.6 – 7.9)
	Pesticide toxicity	> (1 – 1.2) % species affected
	BOD	> (3.1 – 4.5) mg/L
	Chloride	> (43 - 86) mg/L
	Phosphate	> (4.6 – 7.5) mg/L
	Metals toxicity	> (1.1 – 2.5) % species affected
Autumn, Urban	BOD	> (2.02 – 2.75) mg/L
	pH	< (7.7 - 7.8) mg/L
	Chloride	> (40 – 79) mg/L
	Phosphate	> (2.8 - 7.9) mg/L
	Metals toxicity	> (1.1 – 2.5) % species affected
Spring, Agriculture	Ammonia	> (0.15 – 0.55) mg/L
	Chloride	> (43 – 83) mg/L
	Hardness	> (420 – 500) mg/L
	pH	< (7.7 – 8)

Model	Stressor	Impairment association threshold range[1]
Autumn, Agriculture	TSS	> (11.2 – 20.8) mg/L
	Nitrate	> (8.3 – 11.3) mg/L
	Ammonia	> (0.09 – 0.21) mg/L
	TSS	> (20.2 – 41.5) mg/L
	BOD	> (2.5 – 3.8) mg/L
	Hardness	> (295.5 – 419.7) mg/L
	Nitrate	> (9.6 – 13.4) mg/L

Notes: [1]The impairment association threshold is the value range determined in WOE analysis above or below which the odds of site impairment increase (classified as a binary map value = 1 for the WLR model). Stressors are shown ranked by influence for each land use/season model.

4 Discussion

This study has evaluated the applicability of the GIS-based WOE/WLR methodology to the readily available data on surface waters and invertebrate macrofauna for England and Wales, held by the Environment Agency. Although a limited data set has been used, the study, which should be considered as a scoping study, has yielded significant results and map products that may be of use to river basin managers for the purposes of the Water Framework Directive. The model fit evaluations for both the full study area as well as the land use specific WOE/WLR models showed strong explanatory power, consistent with, and in many cases stronger than, previous analyses in other geographic regions (Kapo and Burton, 2006; Kapo *et al*., in Press) The seasonal models for the study area provide geographic predictions of biological impairment based on spatial patterns of stressor variables which allow for more targeted studies. The impairment maps, while informative as a static map, are also interactive GIS maps with stressor rankings associated with each study area grid cell. The result is the ability to perform a targeted assessment with information on location and a list of stressors of concern, based on available data from an established monitoring programme. This is potentially useful not only for river basin characterisation work under the Water Framework Directive, but also in developing appropriately targeted Programmes of Measures.

The most influential variable in the spring season WOE/WLR model for the study area was chloride, which may serve as a proxy variable for surface run-off from spring rain events. Run-off magnitude, particularly urban run-off, has been found to be a highly important factor determining biological impairment in previous WOE/WLR analyses on a geographic region of the United States (Kapo *et al*., in review). The chloride variable in the full study area model may serve as a useful proxy for urban run-off. The examination by specific land use type removes some of the influence of the chloride variable, which suggests a possible use as a land use proxy itself in the full study area model. For example, when examining the data by land use, other stressor variables (Figure 3.9) become stronger predictors of impairment than the chloride variable. While the full study area model provides useful information about impairment location and stressor source, this information is even more refined by further evaluating the data by specific land use. This finding highlights the benefit of taking a land-use specific approach to eco-epidemiological modelling.

Another interesting result when comparing the results in stressor influence between the full study area WOE/WLR seasonal models and the land use specific WOE/WLR models is the influence of metals toxicity. The influence of metals toxicity was higher in urban land use compared with agricultural land use, and higher in the autumn season compared with the spring season. An increased influence of metals in urban areas would be expected because of the greater number of potential sources of metals (industrial, vehicular) in urban land use. There are two possible explanations for the seasonal difference in metals toxicity influence, which may both be correct to some extent. One is a potentially higher overall bioavailability of metals in the autumn season due to seasonal fluctuations in water chemistry (Antunes *et al*., 2007). The metals toxicity variable used in this study considers only hardness-adjusted bioavailable amounts (Posthuma and de Zwart, 2006). Another potential explanation is the increased importance of other factors in the spring season, which outweigh the predictive power of metals stress for macrofauna impairment. This is supported by the relatively higher influence of the pesticide toxicity variable in the urban model for spring, which may simply serve as a proxy for stressors associated with agricultural run-off. This would indicate that in the spring season in urban areas a significant proportion of macrofauna stress may be a result of a combination of urban and agricultural-based stressors. The pesticide toxicity variable was not significant in the agricultural models, however, this is unsurprising given the shortcomings of the modelled pesticide data used, as discussed in Section 3. Improving pesticide toxicity estimates, and predictions of run-off constituents in general, would be of potentially great benefit to future work. Nitrate was found to be a more influential factor in the autumn agricultural land use model compared with the spring model. Nitrate is commonly released to surface waters through crop harvest practices in the autumn season (Vos and van der Putten, 2004).

Cross-comparison of the WOE/WLR method with de Zwart *et al*.'s EPC analysis (2008) showed a strong agreement in stressor identification between the methods, but less agreement in the relative influence of stressor variables. While both methods may have identified a particular variable as a site stressor, in many cases they disagree on the relative significance of a stressor compared with others present. An obvious factor potentially complicating interpretation and contributing to the differences in results is the seasonal split of the data in the WOE/WLR method, and the averaging of EPC site results over all sample years in structuring the comparison. In addition, the inconsistency in stressor influence between the methods is not highly surprising given the different statistical methodologies used. In particular, while the EPC approach visually displays biological impairment based on species loss estimates from RIVPACS, the actual statistical relationships between stressor variables and biological condition are based on species abundance. The WOE/WLR method, in contrast, statistically models the relationship between stressor variables and RIVPACS derived O/E values. It is possible, therefore, that the differences in predicted stressor influence between the methods may in fact reflect that the EPC method gives more weight to stressors with the greatest effect on raw species abundance, and the WOE/WLR method gives more weight to stressors whose presence most increases the probability of obtaining a RIVPACS value below a certain threshold. The general type of stressor (water chemistry, habitat alteration, and so on) may affect how the statistical differences between the methods impact the strength of agreement of the results. For example, the weak correlation between stressor rankings of the methods for the water chemistry variables in this study was similarly found for water chemistry variables in a previous cross-comparison study for fish communities in the state of Ohio, USA (Kapo *et al*., in press). However, in the Ohio study, the site-specific rankings of habitat stressors (which were not evaluated in this current study) showed a strong positive correlation between the methods. A potential explanation requiring further study is that RIVPACS-based O/E and raw species abundance values respond more similarly to habitat alteration than to water chemistry variability.

The disparity between the outputs from these methods causes an obvious problem for interpretation and use of the information by river basin managers. Further work to compare the two approaches more directly is recommended. Careful thought should also be given how the outputs from these methods should be used and interpreted. It is envisaged that the most appropriate application of these methods may be within an evidence-based framework for decision making, alongside other lines of evidence for likely cause of observed biological impact.

It should also be borne in mind that the limited nature of the data used thus far has limited the outputs. Any future work should look to improve the accuracy of some of the existing stressor variables, such as pesticide surface water concentrations. In addition, data on other potentially significant stressor variables such as hydrological modification should be included. In addition, inclusion of other biological information such as diatom and fish data would be a valuable addition, since macroinvertebrates will not be the most sensitive endpoint for all stressors.

5 Conclusions

- The GIS-based WOE/WLR method was successfully applied in the context of a scoping study, to the available biological, chemical, and land use data for England and Wales.
- Outputs from the method included GIS-based maps predicting the location of macro-faunal impairment, together with a ranked list of probable stressors. Visual outputs such as these can be effective communication tools.
- Cross-comparison of the WOE/WLR method with another eco-epidemiological method, the Effect and Probable Cause (EPC) method (de Zwart *et al*., 2008) found that both methods generally agreed on identification of significant stressors at a site, but there were differences between the results. In particular, the relative rank order of stressors was different between each method.
- Differences between the outputs are likely to be because of the different statistical methodologies used. Further work to understand the reasons for the differences is required before outputs can usefully be used in a river basin management context.
- The inclusion of more data on additional stressor variables such as hydromorphological data would increase the usefulness of the method and its outputs and is strongly recommended. Collation of national datasets of sufficient quality and extent for these methods is not a trivial task and the time and effort required should not be underestimated.
- To be of real long-term value, future monitoring programmes should be targeted to ensure that the data collected can be used in eco-epidemiological methods such as those described here and in de Zwart *et al*. (2008).
- Eco-epidemiological approaches such as the WOE/WLR and EPC methods are potentially very useful tools for river basin managers under the Water Framework Directive, especially as part of an evidence-based framework for decision making. Further work should be targeted at developing such a framework.

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List of abbreviations

EPC: Effects and Probable Cause

GIS: Geographic Information Systems

WOE: Weights of Evidence

WLR: Weighted Logistic Regression

RIVPACS: River Invertebrate Prediction and Classification System

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