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Large-scale risk screening of raw water quality in the context of drinking water catchments and integrated response strategies

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ABSTRACT

Water resources provide multiple services, one of the most important the provision of drinking water, conventionally treated before public consumption as potable supplies. With increasing pressures from land use and climate change, there are advantages to be gained from considering raw water quality as a fundamental characteristic of the natural resource, and to anticipate emerging risks within the catchments rather than relying on treatment. This research proposes a large-scale, rapid risk screening of raw water quality based on catchment sensitivity to pressures as prerequisite to a more strategic inclusion of emerging risks in water resource and ecosystem management. Raw water quality observations from 154 surface water catchments in Scotland were investigated to determine the national baseline and to identify current pressures and underlying drivers. Patterns and spatial dependencies were investigated using principal component analysis, redundancy analysis, cluster analysis, and regression trees. These statistical approaches highlight the interaction between intrinsic catchment biophysical properties, land use and climate in characterising water quality risks and identify the focus for prioritising catchment interventions and risk-mitigation in the future. The emphasis on raw water quality will also support an ecosystem-based approach to increase catchment resilience, to ensure long-term supply of good quality drinking water while simultaneously creating wider benefits for society and the environment.

1. Introduction

An essential use of our freshwater ecosystems is for drinking water purposes, with concomitant requirements for water quality to maintain public health (WHO, 2011). In developed countries, achieving statutory requirements for drinking water has conventionally had a technological, end-of-pipe focus on water treatment to manage and mitigate risks to meet regulatory standards. However, mounting pressures on water resources and associated challenges for treatment processes has led to increased interest in more strategic approaches to risk assessment and in particular to the role of targeted interventions that can maintain or improve raw water quality within the catchment (watershed) units that act as water sources (WWAP, 2018). This interest is based upon enhanced awareness of the mutually-reinforcing outcomes that can be gained for the environment, society and economy through healthy, functioning, and resilient ecosystems, together with the notion of raw water quality as being an inherent 'public good' that is associated with multiple benefits through delivery of diverse ecosystem services including provision of drinking water (Everard and McInnes, 2013; Grizzetti et al., 2016; Keeler et al., 2012). Advantages of good raw water quality for water suppliers accrue from reduced treatment costs, reduced carbon emissions and enhanced reliability of source areas for water provision, whilst for other beneficiaries, water quality has a direct link with other goals, notably for biodiversity and amenity value of freshwater ecosystems. Pioneering schemes have consequently been developed through catchment-based partnerships to improve water quality, combining drinking water supply, nature conservation, and amenity agendas, with the aim of achieving not only an economically favourable outcome, but also delivering wider benefits for the environment and society (Appleton, 2002; Morris and Holstead, 2013).

Important as they are, these pioneering schemes typically represent opportunist developments originating in specific catchments due to shared recognition of the need for action based upon known linkages between water quality, habitat restoration and amenity value. This shared recognition often occurs from identification of common problems following degradation of a resource (Margerum and Robinson, 2015). In this contribution, we present the merits of a more systemic and strategic approach to risk assessment based upon large-scale

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characterisation of raw water quality, using this to explore a more proactive policy and operational agenda for catchment source protection at national scale that includes both existing and emergent risks. The strategic approach aims to improve awareness of spatial and temporal dimensions of risk together with the role of resilient ecosystems in mitigating that risk, and therefore to inform policy and planned interventions at a scale above that of opportunist local catchment schemes. Interventions may therefore be designed in response to existing water resource pressures (e.g. increased demand; land use intensification) but also to anticipate and counteract additional emergent risks, notably due to climate change.

At country-level, water resource planners develop strategic initiatives to secure a safe and reliable water supply, including safeguarding raw water quality (Le Moigne et al., 1994). Risk assessment for water quality is standard practice in many countries (Hrudey et al., 2006), as informed by regular monitoring of resources and underpinned by statutory regulation, but risk management is normally based upon existing recognised hazards and consequent risks in specific catchments, together with established procedures to react to detected changes in risk levels. Risks can propagate from existing geochemical mineralogical hazards associated with specific rocks and sediments, and from the presence of soil organic particulate, biogeochemical, or microbiological contaminants (bacteria, protozoa etc.). In each case, regulatory standards for drinking water define risk tolerance in terms of safe concentrations of potential contaminants, as formalised both internationally (WHO, 2011) and through national policy. In addition, raw water quality is an important constituent of other regulatory policies, including for bathing water and aquatic biodiversity. Recognition that multiple policy instruments can be in conflict when defined in isolation has led to a shift towards finding more integrated solutions, and in particular to the role of the Ecosystem Approach in providing a more coherent strategy for sustainability goals (Brown and Everard, 2015). In the water sector, this has led to development of more holistic policy frameworks which aim to integrate regulatory instruments within a common structure, as exemplified by the EU Water Framework Directive (Directive 2000/60/EC) which has defined objectives based upon characterisation of good ecological and chemical status of water bodies (Everard, 2011; Vlachopoulou et al., 2014).

Land use changes associated with intensification, and ongoing climate change, are increasing pressures on natural hydrological and biogeochemical processes. Direct effects arise from modified soil moisture levels and streamflows, erosion, increased carbon fluxes, declining ecosystem productivity and ecosystem resilience, with indirect negative impacts on pollutant loads and water quality expected to increase in the future (Delpla et al., 2009). These drivers and pressures will further challenge existing treatment infrastructure and purification techniques, and lead to an increase in effort and costs for treating water to meet standards (Ritson et al., 2014). Arguments, such as ‘the uniqueness of place’ (Beven, 2000), suggests that efforts to model water quality risks for individual catchments will only have limited utility without a broader analytical framework in which to contextualise results and derive general inferences needed to develop catchment management plans within the framework of strategic policy goals for water resources (Everard and McInnes, 2013). Larger-scale approaches can infer specific water quality parameters based upon catchment characteristics (Davies and Neal, 2004; Rothwell et al., 2010), aided by use of statistical analysis to improve understanding of underlying drivers (e.g. Selle et al., 2013; Shen et al., 2011; Shi et al., 2017). Challenges and advantages of finding catchment commonalities and typologies are increasingly recognised in hydrological sciences, highlighting the need for large-scale approaches and pooling of datasets to help discriminate and categorise complex cause-effect relationships occurring in catchments in a non-stationary climate (e.g. Beven, 2016; Kundzewicz, 2018; Wagener et al., 2007).

The combination of scale, complexity and changing drivers thus identifies scope for developing a risk screening approach to catchment characterisation at strategic level. Screening seeks to identify key catchment properties and their spatial characteristics in relation to water quality parameters, and hence those catchments that are at higher risk in terms of loss of quality, both at present, and in the future as dynamic catchment properties are modified. The underlying rationale is that this procedure can be a basis for catchment prioritization in terms of: monitoring and research to understand processes in more detail; mitigation and restoration measures that increase resilience; stakeholder engagement to better co-ordinate anticipatory adaptation strategies based upon a shared recognition of change.

The basis of risk screening is to investigate current impacts, as recorded through monitoring data, and their association with existing pressures on water resources as well as catchment sensitivity to different types of risks. The current range of risk as exhibited by raw water quality parameters can therefore be examined in relation to catchment characteristics in order to characterise key risk relations and their spatial and temporal dimensions. This strategic approach and identification of vulnerable catchments then provides a baseline against which additional stresses, notably from increased exposure to changing hydroclimate drivers (e.g. modified precipitation regime) or land use change can be referenced and precautionary actions adopted to maintain or enhance raw water quality.

The present study applies this risk screening approach for drinking water catchments in Scotland by analysing relationships between catchment characteristics and observed raw water quality parameters. Scotland provides an excellent case study because of its heterogenous landscape, diverse water resource management approaches, and policy recognition for improved risk-based approaches to help secure and maximise multiple benefits in a changing world (Scottish Government, 2011; Water Resources (Scotland) Act 2013). Screening of drinking water catchments therefore aims to identify those at greatest risk by identifying commonalities in characteristics and response, and hence key risk factors to be addressed, including response strategies that augment both research and monitoring, and enhance ecosystem resilience.

2. Methods

2.1. Study catchments

Across Scotland, 154 catchments were analysed as sources for reservoir, lake and river intakes used by the national public supplier, Scottish Water. Each catchment was characterised in terms of natural conditions, as well as anthropogenic pressures using public data sets (Table S1). Characteristics were chosen as representing potential influences on water quality. Topography, described by proportions of steep/gentle slopes or relief ratio (elevation difference per length of catchment), influences water runoff speed and thus mobilisation of particles. Bedrock geology as well as soil properties can influence mineral concentration, pH and hydrological pathways. Land use and management can be sources of contaminants or alter catchment hydrology. Temperature influences microbial activity and vegetation growth which can impact water quality, whilst precipitation patterns determine soil erosion, water quantity and relative dilution/concentration of pollutants, and induce seasonal catchment changes in hydrological pathways.

The great majority of catchments are very small (median size $3.84\,km^2$), with a few exceptions (9 catchments $>100\ km^2$, and $3 > 1000\ km^2$). Mean elevation peaks at between 250–300 m. Slopes are predominantly moderate (between 4°–15°); however, some catchments also have high proportions of steep slopes (above 15°), or gentle slopes (below 4°). Most catchments are dominated by semi-natural habitat, especially heathland, while extensive coniferous forest and improved grassland also feature in several catchments. There are low percentages of urban areas (maximum 2.15%), and low arable area cover (only five catchments with $>10\%$, maximum 40.26%).

Scotland has a heterogeneous geology, but most catchments are underlain by metamorphic and igneous lithologies. A smaller number occur on sedimentary series (mainly sandstone), whilst fewer still feature calcareous strata and only one with 100% limestone, broadly consistent with national coverage. Many catchments have a high percentage of peat soils (histosols) or those with a significant surface organic horizon (e.g. peaty gleysols), because of the common presence of such soils in the uplands, meaning high proportions of soil organic carbon.

Mean temperatures and total precipitation reflect the oceanic temperate climate of Scotland dominated by Atlantic weather systems. There is a pronounced west-east gradient in total rainfall with catchments in the west mainly experiencing higher rainfall than catchments in the east, also reflecting additional orographic influences.

2.2. Water quality data

Data regarding eight water quality parameters routinely monitored in accordance with regulatory requirements (aluminium, colour, pH, iron, manganese, presumptive coliforms, presumptive *E. coli*, and turbidity) were included in the analysis, provided by Scottish Water for years 2011 – 2016. Sampling regimes vary per catchment with parameters being sampled from every three months to every week according to the assumed level of risk, resulting in a minimum of 18 samples from one catchment for the least sampled parameters (pH and bacteria) up to a maximum of 238 samples from catchments on higher frequency sampling for some parameters (colour, iron, manganese, turbidity). Average sample numbers were 93 (aluminium), 99 (colour, turbidity), 100 (iron, manganese), 39 (pH) and 38 (coliform, *E. coli*) per catchment.

2.3. Data analysis

Four statistical approaches were applied in combination with the aim of inferring key relationships within this large multivariate dataset: principal component analysis (PCA), cluster analysis, redundancy analysis (RDA), and regression-tree type analysis. Consistent with the risk screening rationale, the analysis used these techniques in an exploratory mode to help infer key data relationships and their interpretation in terms of causative risk factors.

PCA is a widely used approach to analyse water quality variability (Li et al., 2013; Shen et al., 2011) and allowed to examine both variability in water quality between catchments and associative patterns in the multivariate data. It determined optimal linear combinations (principal components, PCs) of the water quality parameters that explain most data variability. PCs often reflect key processes that are not directly observable in the original data (Selle et al., 2013). Information about catchment characteristics was superimposed to the PCA solution as supplementary variables. This aided an understanding of the primary associations between catchment characteristics and quality parameters allowing initial insights into prospective relationships that define catchment sensitivity.

RDA is a multivariate statistical technique which combines linear regression and PCA to examine the relationships between two multivariate data sets, explicitly assuming that one corresponds to response variables and the other to explanatory variables. This method has found varied applications in water quality research (e.g. Ding et al., 2016; Shi et al., 2017). Here, it was used to simultaneously examine the influence of a set of catchment characteristics on water quality parameters, so that it helped to summarise the variability in the water quality variables that can be explained by selected catchment characteristics.

Cluster analysis was employed to identify groups of catchments showing homogenous profiles of water quality (Shen et al., 2011; Singh et al., 2004). Analysing clusters at national level helped to interpret water quality scale issues including exploration of geographic patterns of catchment sensitivity associated with different risk factors.

Finally, multi-target predictive clustering trees (MTPCTs; Struyf et al., 2011), were fitted to further test associations between individual water quality variables and catchment characteristics. Advantages of tree-based regression analysis include being non-parametric models allowing recursive data partitioning which is well-suited to deal with complex non-linear relationships and high-order interactions, is generally less sensitive to outliers, and encapsulates results in an intuitive and easy to interpret hierarchical structure to aid decision-making (Breiman et al., 1984). They are especially suitable for analysing patterns in large noisy datasets (Atkins et al., 2007). MTPCTs generalise ordinary regression trees by estimating expected values for more than one variable at a time and have been shown to be effective for identifying important parameters from diverse attributes (Demšar et al., 2006). MTPCT allowed to jointly consider average concentrations (i.e. catchment medians) as well as extremes (i.e. 95th percentiles), producing an estimated value for each depending on catchment characteristics as explanatory variables.

Statistical data analyses and graphical representations were undertaken in R v3.4 (R Core Team, 2018). Spearman's rank correlations tests provided a robust method suitable for non-normally distributed data, to initially investigate individual relationships between catchment medians. Water quality sample data were then log transformed to normalise distributions with catchment medians and 95th percentiles used in subsequent analyses. Medians summarised average water quality values per catchment as input for PCA. Catchment characteristics were projected onto the biplot space spanned by the first two PCs to aid interpretation of water quality relationships. Their biplot coordinates were derived from correlation with the PCs (Graffelman and Aluja-Banet, 2003). During the RDA, non-significant catchment characteristics were removed from the model through backward elimination, and two further variables (steep slope and gentle slope) were removed manually to reduce collinearity (topography being represented as relief ratio). Variance inflation factors (VIF) were derived to assess multicollinearity. For the cluster analysis, the partitioning around medoids (PAM; Kaufman and Rousseeuw, 1990) clustering algorithm was used with the standardized (z-transformed) catchment medians, and their dissimilarity measured using Euclidean distances. PAM is a partitional clustering technique, similar to k-means algorithm, but using actual data points as cluster centres, which minimises influence of outlying observations. Clustering structure quality was assessed using the average silhouette width measure (Kodinariya and Makwana, 2013) with number (k) of clusters determined through best silhouette width. Overall differences between clusters were tested for statistical significance using the Kruskal-Wallis test. Pairwise differences between clusters were tested using the Wilcoxon test. The software package Clus (Struyf et al., 2011) was used to produce eight MTPCTs with their performance assessed using root mean square error (RMSE) and R^2 values from training and testing using 10-fold cross-validation.

3. Results

3.1. Statistical summary of water quality parameters

Summary statistics of catchment water quality data revealed strong skewness (Table S2), with most of the parameters falling within the lower concentration range and a few branching up to very high concentrations; apart from pH which is log-scale. Most catchments had source concentrations below consumer drinking water standards for aluminium, iron, manganese, and turbidity (0.2, 0.2, and 0.05 mg/l and 4 NTU respectively (The Public Water Supplies (Scotland) Regulations 2014)). Most catchments had colour concentrations above the 20 mg/l Pt/Co drinking water standard, showing a widespread need for colour treatment in Scotland. For pH, catchments falling outside the required range (6.5–9.5) were more acidic, with values down to 5.5. Coliform bacteria were usually present in drinking water, making disinfection a necessary step in every treatment works.

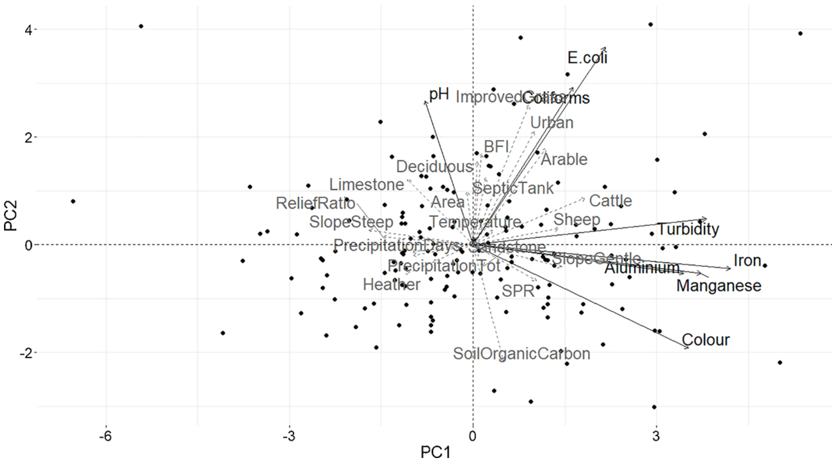

Fig. 1. PCA biplot: catchment water quality parameters (black rays), catchment characteristics as supplementary variables (grey dashed rays), and individual catchments (points).

Spearman's correlations indicated relatively strong ($r > 0.6$) monotonic relationships between iron and colour, iron and manganese, iron and turbidity, manganese and turbidity, and coliform and *E. coli*, and moderate ($r > 0.4$) monotonic relationships between aluminium and colour, aluminium and iron, aluminium and manganese, aluminium and turbidity, colour and manganese, and colour and turbidity.

3.2. PCA

The first three PCs explained 80% data variance (46% PC1, 20% PC2, and 14% PC3). The first two PCs' biplot (Fig. 1) revealed most catchments are relatively evenly scattered around the origin. PC1 was most associated with levels of turbidity, metals and colour; PC2 with pH, coliform and *E. coli* (Table S3). Catchments located towards the upper part of Fig. 1 were associated with increasing values of coliform and *E. coli*, and higher proportions of improved grassland, arable and urban cover, whereas those placed more toward the right-hand side presented higher values of metals, colour and turbidity, associated with reduced precipitation, increased livestock densities, and gentler reliefs. Toward the lower right corner, catchments were mostly characterised by increasing values in colour and decreasing pH, correlated with topsoil organic carbon content.

3.3. RDA

Through elimination of non-significant variables and collinearity analysis, a reduced set of catchment characteristics (relief ratio, Baseflow Index, topsoil organic carbon content, improved grassland, arable, and urban land cover, cattle and sheep density, and precipitation days >10 mm) was included in the RDA model as constraining variables. VIFs ranged from 1.3 to 2.3, hence collinearity was not considered to be a confounding factor (threshold value 10: Alin, 2010)). The first two RDA axes constrained 53% and 32% respectively of total variance of water quality parameters, which corresponded to 17% and 10% of the overall variance.

The RDA triplot (Fig. 2) showed all water quality variables loaded positively the first RDA axis, although colour was negligible. Improved grassland, arable and urban cover, sheep and cattle density, and BFI also contributed positively to RDA1, indicating increases in these variables matched increased concentrations in bacteria, turbidity and metal parameters, whilst a negative relationship was shown for relief ratio, soil organic carbon and precipitation. For RDA2, colour, iron and manganese were strongly negatively associated, while pH was strongly positively associated, meaning catchments with higher concentrations in colour, iron and manganese were usually more acidic. Average topsoil organic carbon content was strongly negatively associated with

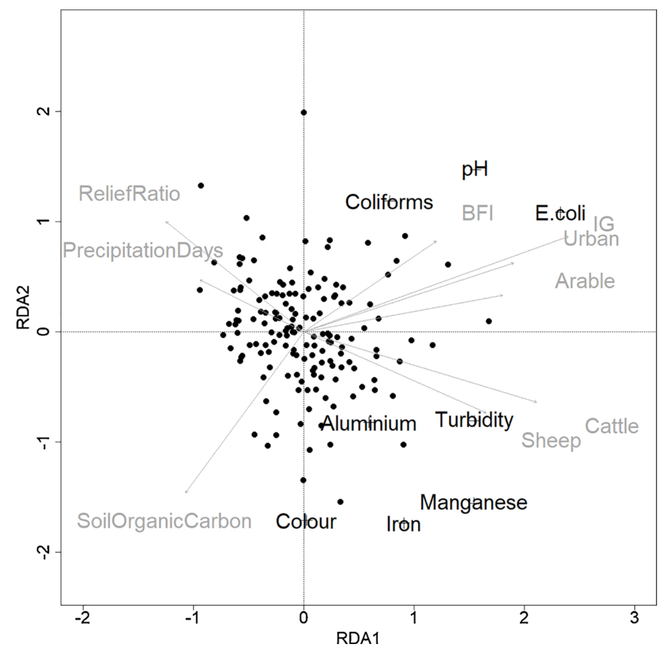

Fig. 2. RDA triplot: water quality parameters (black), catchment characteristics as constraints (grey rays), and individual catchments (points). IG - Improved grassland.

RDA2 whilst relief ration was positively associated, confirming colour problems as most severe on organic soils and gentler reliefs. While agricultural and urban land uses, to a lesser extent, associated positively with RD2, sheep and cattle density corresponded negatively with these two variables, showing them to be good candidate explanatory factors for colour, iron, manganese and turbidity (Table S4).

3.4. Cluster analysis

Using catchment medians for PAM-based clustering produced five clusters with an overall weak clustering structure (average silhouette width 0.21), and with unequal cluster sizes (63, 40, 30, 16, 5 in clusters 1–5 respectively). Water quality parameters (Fig. 3) were overall statistically significantly different between clusters ($p < .001$). There were also significant ($p < .001$) differences between catchment characteristics per cluster (Fig. 3), notably in topography (relief ratio), precipitation, topsoil organic carbon content, cattle density, and arable and improved grassland cover.

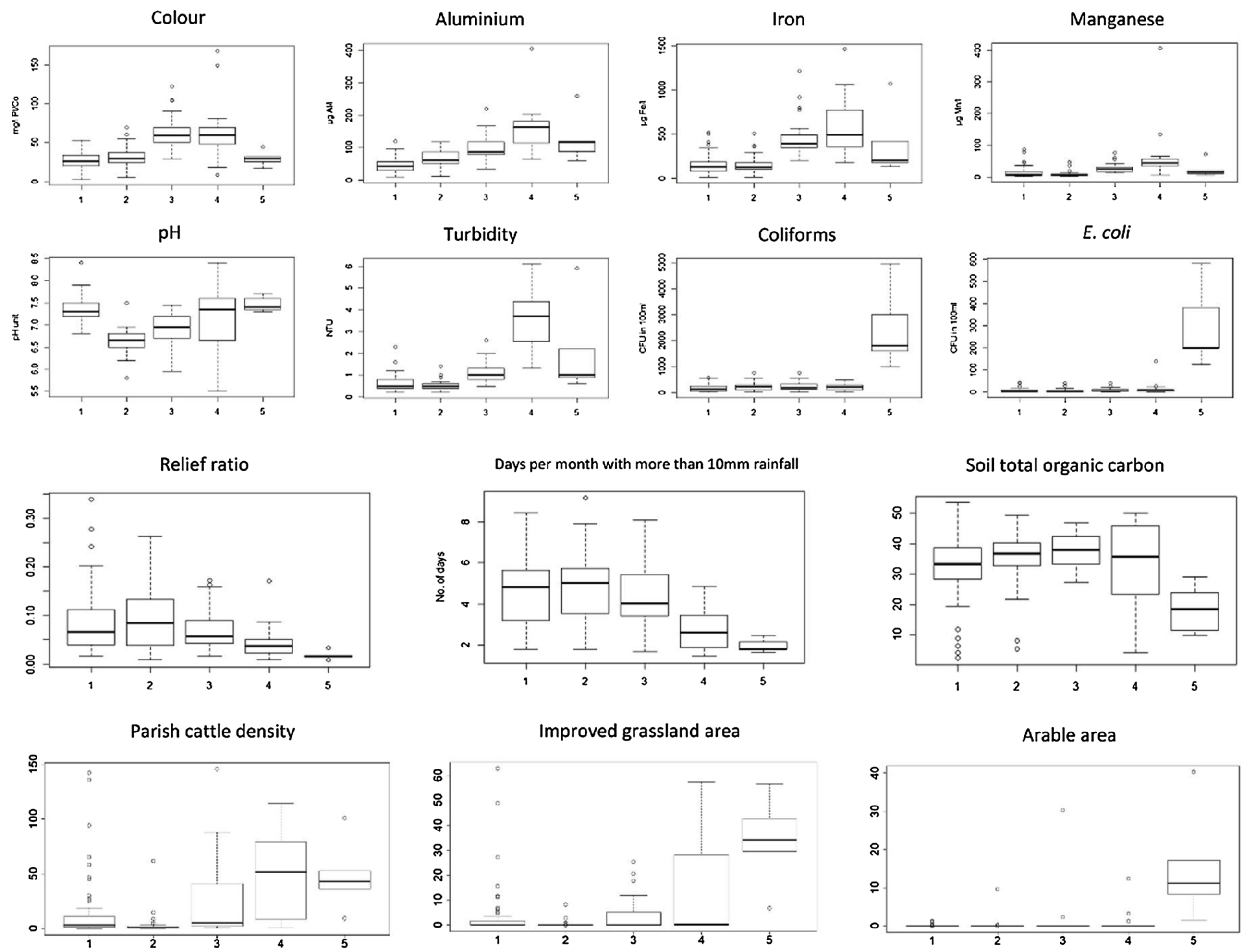

Fig. 3. Boxplots of water quality parameters and catchment characteristics per cluster.

Examining the geographic distribution (Fig. 4), cluster 2 occurred predominantly in the Northwest, cluster 3 mainly along the West coast, cluster 4 in the East, in the South and on Orkney, and cluster 5 was restricted to the Northeast. This broadly corresponds to a basic distinction that can be made between catchments in the west of Scotland, mainly characterised by steeper slopes, impermeable bedrock, high precipitation, and dominant semi-natural land cover; and lowland areas mainly in the east and south with gentler slopes, less precipitation and land uses that include more intensive agriculture. However, there were also locations where catchments in different cluster groups were spatially adjacent, which suggests local-scale factors add further variability of catchment behaviour.

3.5. Regression tree modelling

MTPCTs showed differences in RSME and R^2 values between training and test sets (Table 1), which indicates overfitting to the training set, and their purely predictive capability was low. However, the aim of this study was to understand key explanatory factors and the results of the models are useful to explore the relationships between water quality variables and catchment characteristics.

The MTPCT for aluminium featured cattle density and coniferous forest cover as separators, with concentrations being higher where cattle density is higher or coniferous forest covers more than half of the catchment. Some catchments were separated showing especially larger ranges of concentrations where mean annual temperature or precipitation is lower. The MTPCT for colour indicated that catchments with higher soil organic carbon content would yield higher colour concentrations. The same could be seen for iron, with catchments showing higher concentrations where topsoil organic carbon content is higher, or with higher cattle density. The MTPCT for manganese only separated two catchments with higher concentrations containing the highest sheep densities. PH values were highest in catchments with more than 25% improved grassland, and low where soil organic carbon is higher, or baseflow index lower. The turbidity model showed highest values for catchments with high improved grassland cover, or high in sandstone bedrock. Turbidity values were also higher for catchments with cattle or sheep, or if soils have a higher surface runoff ratio. Coliform and *E. coli* MTPCTs separated two catchments with urban area cover and highest concentrations first. The *E. coli* tree then also identified catchments with septic tanks as having higher concentrations.

4. Discussion

4.1. Water quality, catchment variability and risk factors

Drinking water catchments analysed reflected the variety of environmental conditions found across Scotland. Many showed similarity in baseline raw water quality characteristics with predominantly low concentrations of aluminium, iron, manganese, and turbidity, although there was a wide variability in pH.

In Scotland, high concentrations in aluminium, iron, manganese and dissolved organic carbon (DOC) are usually associated with acidic pH and organic, poorly drained peat soils, as solubility increases at low pH and under anaerobic conditions (Abesser et al., 2006). The colour and high topsoil organic carbon relationship was a pattern that emerged in

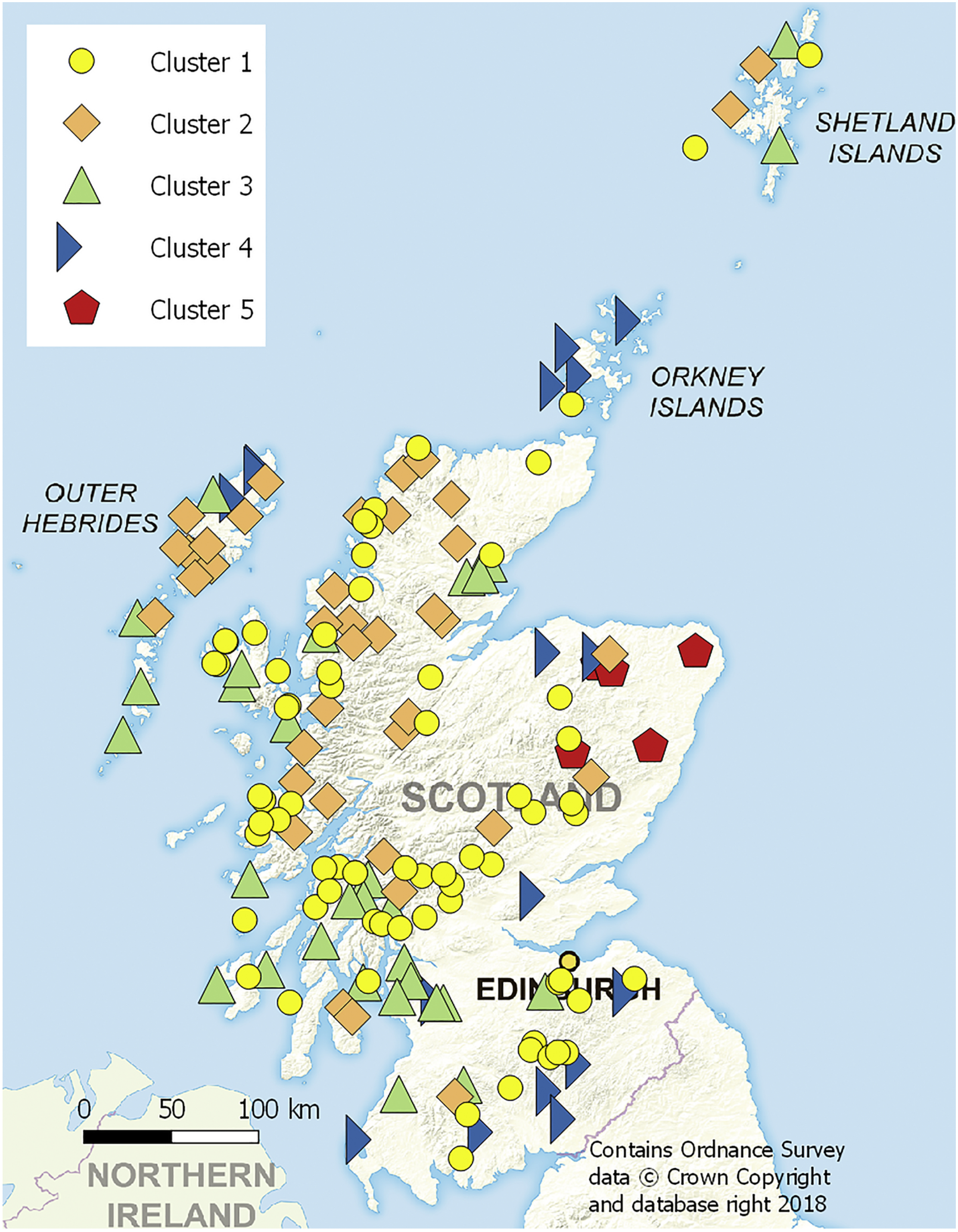

Fig. 4. Spatial distribution of catchment clusters.

all methods, especially in the RDA where the second RDA axis showed that colour, as well as iron and manganese, related to high average of topsoil organic content, low pH and gentler reliefs. Therefore, more acidic, peaty upland catchments prone to water-logged conditions can generally be identified as candidate catchments for higher colour risk. Cluster analysis suggested that there may also be local factors leading to varying concentrations in colour and metal parameters, potentially due to catchment geology (which would not be sufficiently represented through percentage of limestone and sandstone cover) or a greater catchment extent of degraded or eroded peat. The RDA identified influence of cattle and sheep density, which supports a possible relationship to peat degradation.

Similarly, land use variables clearly showed a positive association with the first RDA axis, which mainly related to metal variables alongside turbidity and *E. coli*, suggesting a relationship with more intensive forms of land use also for these parameters. Cattle and sheep densities appeared in the MTPCTs for aluminium, iron, manganese, and turbidity, maybe pointing towards erosion related processes. Higher SPR of the soil also associated to higher turbidity, which can occur when rainfall quickly runs off the surface, picking up particles from bare and disturbed ground. The coniferous forest cover in the aluminium MTPCT could point towards similar processes of disturbance through forestry, or be related to acidification of soils. Interestingly, coniferous forest cover was not picked up as significant in the other methods, which could indicate a varying influence of forestry in combination with other characteristics and management.

Bacteria concentrations correlated well with land use, especially improved grassland, arable and urban areas. Perhaps surprisingly, improved grassland or livestock densities were not stronger explanatory variables for these parameters in the MTPCTs. Neill et al. (2018) found that especially in small catchments, the extent of arable or pasture land was not a good predictor for *E. coli* concentration, due to greater influence of point sources over diffuse sources. Septic tanks as point sources were included in the *E. coli* MTPCT, and the number of septic tanks also correlated with PC2, but there are only few catchments with septic tanks, and they were not included as a significant variable in the RDA. Catchments with urban cover and septic tanks are usually the ones that have higher percentages of agriculture, so there may be an overlapping effect of direct influences from arable agriculture and livestock, and other factors associated with catchments more suitable for

Table 1

MTPCTs per water quality parameter. Predictors used were relief ratio, percentage of limestone bedrock and of sandstone bedrock, average value for topsoil organic carbon content (TOC), average Baseflow Index (BFI), average Surface Percentage Runoff (SPR), percentage coniferous forest, deciduous forest, arable, improved grassland, urban and heathland area cover, average density per parish 2013–2017 of cattle and of sheep, number of septic tanks in the catchment, mean annual temperature, and mean monthly rainfall. 'yes' and 'no' refer to the condition above, leading to a new condition or the predicted median and 95th percentile values in [], followed by the number of catchments falling within this prediction.

<table>
<tr><th rowspan="2">MTPCT – pruned</th><th rowspan="2">Standard deviation of complete data set</th><th colspan="2">RSME</th><th colspan="2">R^2</th></tr>
<tr><th>Training</th><th>Testing</th><th>Training</th><th>Testing</th></tr>
<tr><td>Aluminium:
Cattle > 46.9
+--yes: [131.85, 738.2]: 24
+--no: Coniferous > 50.1
+--yes: [124.5, 334.13]: 6
+--no: MeanTemperature > 5.01
+--yes: MeanMonthlyRainfall > 82.1
| +--yes: [59.46, 166.24]: 113
| +--no: [98.06, 398.03]: 8
+--no: [109.83, 732.8]: 3</td><td>[51.81, 408.18]</td><td>[42.9, 344.28]</td><td>[53.68, 430.73]</td><td>[0.31, 0.28]</td><td>[0.06, 0.05]</td></tr>
<tr><td>Colour :
OrganicCarbonContent > 40.24
+--yes: [55.41, 122.47]: 37
+--no: [33.75, 65.84]: 117</td><td>[24.93, 55.04]</td><td>[23.06, 49.23]</td><td>[25.68, 55.99]</td><td>[0.14, 0.19]</td><td>[0.02, 0.04]</td></tr>
<tr><td>Iron:
OrganicCarbonContent > 45.33
+--yes: [640.25, 1886.08]: 12
+--no: Cattle > 46.9
+--yes: [389.2, 1785.77]: 20
+--no: [210.81, 713.61]: 122</td><td>[243.87, 1185.41]</td><td>[209.27, 1092.17]</td><td>[251.52, 1228.4]</td><td>[0.26, 0.15]</td><td>[0.03, 0.01]</td></tr>
<tr><td>Manganese:
Sheep > 323.1
+--yes: [218.75, 3049.75]: 2
+--no: [19.53, 183.03]: 152</td><td>[36.99, 688.91]</td><td>[29.16, 605.12]</td><td>[42.39, 765.07]</td><td>[0.37, 0.22]</td><td>[0.005, 0.002]</td></tr>
<tr><td>Turbidity:
ImprovedGrass> 27.1
+--yes: [3.19, 32.44]: 11
+--no: GeologySandstone > 95.54
+--yes: [1.71, 8.74]: 18
+--no: Heather > 0.0
+--yes: Cattle > 9.1
| +--yes: [1.05, 3.46]: 27
| +--no: ReliefRatio > 0.062
| +--yes: [0.5, 1.75]: 55
| +--no: Sheep > 35.4
| +--yes: BFI > 0.35
| | +--yes: [1.25, 5.04]: 5
| | +--no: [0.75, 2.41]: 14
| +--no: [0.48, 1.49]: 18</td><td>[1.09, 13.12]</td><td>[0.72, 10.14]</td><td>[1.08, 17.57]</td><td>[0.57, 0.4]</td><td>[0.18, 0.06]</td></tr>
<tr><td>+--no: SPR > 49.86
+--yes: [4.35, 28.34]: 2
+--no: [0.73, 2.9]: 4</td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>pH:
ImprovedGrass > 25.44
+--yes: [7.76, 8.17]: 12
+--no: Cattle > 1.6
+--yes: OrganicCarbonContent > 46.77
| +--yes: [6.4, 6.8]: 4
| +--no: MeanMonthlyRainfall > 79.59
| +--yes: [7.2, 7.53]: 84
| +--no: [7.35, 9.19]: 2
+--no: BFI > 0.14
+--yes: BFI > 0.16
| +--yes: [6.73, 7.14]: 39
| +--no: [5.87, 6.5]: 3
+--no: BFI > 0.02
+--yes: [6.5, 9.94]: 2
+--no: [7.05, 7.35]: 8</td><td>[0.49, 0.58]</td><td>[0.35, 0.35]</td><td>[0.49, 0.7]</td><td>[0.5, 0.64]</td><td>[0.12, 0.01]</td></tr>
<tr><td>Coliform:
Urban > 1.02
+--yes: [3275, 15250]: 2
+--no: [239.81, 1985.01]: 152</td><td>[497.98, 2507.48]</td><td>[358.17, 1997.77]</td><td>[594.19, 2768.92]</td><td>[0.48, 0.36]</td><td>[0.03, 0.02]</td></tr>
<tr><td>E. coli:
Urban > 1.02
+--yes: [390, 2815]: 2
+--no: SepticTank > 0.0
+--yes: [126.42, 1030.67]: 6
+--no: MeanMonthlyRainfall > 77.08
+--yes: MeanMonthlyRainfall > 234.12
| +--yes: [8.63, 643.25]: 4
| +--no: [7.85, 114.72]: 139
+--no: [16.5, 1014]: 3</td><td>[60.93, 528.8]</td><td>[36.58, 371.24]</td><td>[74.93, 629.1]</td><td>[0.64, 0.5]</td><td>[0.04, 0.03]</td></tr>
</table>

(*continued on next page*)

Table 1 (*continued*)

+--no: SPR > 49.86 +--yes: [4.35, 28.34]: 2 +--no: [0.73, 2.9]: 4					
pH: ImprovedGrass > 25.44 +--yes: [7.76, 8.17]: 12 +--no: Cattle > 1.6 +--yes: OrganicCarbonContent > 46.77 | +--yes: [6.4, 6.8]: 4 | +--no: MeanMonthlyRainfall > 79.59 | +--yes: [7.2, 7.53]: 84 | +--no: [7.35, 9.19]: 2 +--no: BFI > 0.14 +--yes: BFI > 0.16 | +--yes: [6.73, 7.14]: 39 | +--no: [5.87, 6.5]: 3 +--no: BFI > 0.02 +--yes: [6.5, 9.94]: 2 +--no: [7.05, 7.35]: 8	[0.49, 0.58]	[0.35, 0.35]	[0.49, 0.7]	[0.5, 0.64]	[0.12, 0.01]
Coliform: Urban > 1.02 +--yes: [3275, 15250]: 2 +--no: [239.81, 1985.01]: 152	[497.98, 2507.48]	[358.17, 1997.77]	[594.19, 2768.92]	[0.48, 0.36]	[0.03, 0.02]
***E. coli*:** Urban > 1.02 +--yes: [390, 2815]: 2 +--no: SepticTank > 0.0 +--yes: [126.42, 1030.67]: 6 +--no: MeanMonthlyRainfall > 77.08 +--yes: MeanMonthlyRainfall > 234.12 | +--yes: [8.63, 643.25]: 4 | +--no: [7.85, 114.72]: 139 +--no: [16.5, 1014]: 3	[60.93, 528.8]	[36.58, 371.24]	[74.93, 629.1]	[0.64, 0.5]	[0.04, 0.03]

these land uses.

4.2. Implications for risk management

Some areas of Scotland, especially the transition zones between uplands and lowlands, are anticipated to become more suitable for agricultural intensification through climate change because constraints are reduced in a warmer climate (Brown et al., 2010). Evidence suggests that recent climate warming has already improved agricultural land capability, and in combination with socioeconomic factors this may be associated with recent changes in land use, such as shifts towards autumn-sown rather than spring-sown crops or increased outdoor overwintering of livestock (Brown and Castellazzi, 2014). Our analysis highlights risks especially regarding bacterial contamination from agriculture or associated factors, so the next step in risk screening for water quality will be to use the catchments identified in this large-scale analysis to further investigate the causes for higher levels of bacteria. Risk screening is therefore being used to identify both vulnerable and potentially vulnerable catchments including those where forward projections suggest a higher likelihood of further land use change that may impact water quality.

Colour concentrations tend to be above the potable drinking water standard in Scottish water sources. There are indications that DOC release from Scottish peatlands will rise further (Evans et al., 2005; Ritson et al., 2014; Sawicka et al., 2017), which may be exacerbated by a changing climate, linking projected heavier rainfall (ASC, 2016; Burt and Howden, 2013) with increased erosion and runoff rates (Li et al., 2016). While generally confirming that catchments with acidic, highly organic soils are high risk for colour production, more specific risk factors are difficult to disentangle looking at percentiles alone. Further work to explore time and event-based relationships will be needed to allow further conclusions on which conditions (such as topography, peat condition, and land uses) further contribute to catchment vulnerability in terms of colour production.

Concentrations for all parameters investigated suggested an inverse relationship with catchment precipitation values, indicating an important relationship with water quantity, and that risks appear to be greater for catchments that receive less precipitation, potentially due to a reduced dilution of contaminants. This needs to be further explored, especially because its potential importance is emphasised by climate change projections for an increased frequency of drier summers in the UK (Lowe et al., 2018).

4.3. Role of risk-screening

A foundation for strategic-level risk assessment was produced by combining different statistical approaches which provided complementary information. PCA showed overall trends and controls in the water quality data and allowed first identification of catchments with distinct water quality profiles. While many catchments showed elevated concentrations for all or a suite of parameters in the raw data, the PCA clearly showed a decoupling of parameters or groups of parameters (microbial, colour, and metals and turbidity). RDA helped to establish explanatory roles of catchment characteristics. The cluster analysis used the water quality patterns to separate catchments with different profiles. A spatial perspective was added which pointed towards influences acting on a national scale, as well as to the potential importance of local conditions that govern water quality. Lastly, the MTPCTs identified the most important characteristics associated with individual water quality parameters and facilitated neater interpretation of the influence of local variations.

Considering the variety and complexity of catchments, and the broad-scale analysis, it is unsurprising that some relationships between raw water quality and catchment characteristics remain unresolved. Summarising on medians, rather than investigating all sampling points per catchment individually, might mask relevant data variability within a catchment and fail to capture differences between catchments for example in response to extreme events. The different sampling regimes also mean that in catchments with lower sampling frequencies, extremes are likely missed, while in catchments with higher frequency sampling, a slight bias to high values may exist from reactive sampling following high concentrations, therefore exaggerating differences in baseline concentrations, although the use of medians as a robust measure helped to minimise the potential bias. Catchments are predominantly small, so relating catchment characteristics to water quality becomes more challenging as correlations seem to become weaker at this scale, and there is high spatial and temporal diversity in headwater streams (Abbott et al., 2017). For some catchment characteristics (e.g. geology and geochemistry) small catchment size identifies a need for high-resolution data beyond that available through national-scale surveys. Responses vary depending on local factors: reservoirs and lakes for example will buffer high concentrations following extreme events, so similar catchment responses may show a different outcome in the observed water quality parameter depending on water body type. Finally, catchment profiles could look similar but with different spatial land cover distributions or other local properties relative to the water sample site, and consequently show very different water quality outcomes to similar pressures. A more detailed exploration of catchment conditions together with a stronger focus on catchment responses to extreme events is necessary to understand what makes catchments vulnerable to pressures, which allows a better understanding of how catchment will react to changes in these pressures. The next stage in risk screening should therefore be to investigate confounding effects and improve the quality of data for those priority catchments identified at higher risk.

Identification of high-risk catchments also acts to prioritise the need for co-ordinated intervention. Risk screening results can play an important role in facilitating awareness and deliberation of how best to co-ordinate actions to deliver common objectives on water quality outcomes. The crucial role of land use and land management has been highlighted in the present study in terms of increased risk of resource degradation. For water suppliers, it can identify the need to enhance collaboration with land managers and resource users, and the need to adopt more coherent sampling to support similar analysis and simplify pooling of data. Risk screening results can help further promote the key role of raw water quality in indicating ecosystem health and resilience. Good management practice linking land use and water sectors is likely to become increasingly important as climate change brings further shifts in extreme rainfall events that transfer pollutants to water bodies and low flow episodes that increase pollutant concentrations beyond safe limits (Brown, 2018).

5. Conclusion

A strategic risk-screening approach to raw water quality that combined four different statistical analyses has been developed and applied in Scotland. Screening has identified dominant risk factors and higher-risk catchments that act as priorities for more detailed analysis and improved sampling. Risks are particularly highlighted for colour and bacteriological quality parameters, strongly linked to management of organic soils and agriculture, although other interacting risk factors confound a simple interpretation. In both cases, risks are likely to be further modified by land use change and climate change, which identifies the need for targeted and co-ordinated interventions to better manage risk.

Declarations of interest

None

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Appendix A. Supplementary data

Supplementary material related to this article can be found, in the online version, at doi:https://doi.org/10.1016/j.envsci.2019.05.012.

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