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Methods for detecting change in hydrochemical time series in response to targeted pollutant mitigation in river catchments

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SUMMARY

Detecting changes in catchment hydrochemistry driven by targeted pollutant mitigation is high on the scientific agenda, following the introduction of the European Union Water Framework Directive. Previous research has shown that understanding natural variability in hydrochemistry time series is vital if changes due to mitigation are to be detected. In order for change to be detected in a statistically robust manner, the data analysis methods need careful consideration. Previous work has shown that erroneous results have often been obtained when statistical analyses have been carried out despite the associated test assumptions not being met. This paper discusses the principal data issues which must be considered when analysing hydrochemical datasets, including non-normality and non-stationarity. A range of statistical techniques is discussed which could be used to detect gradual or abrupt changes in hydrochemistry, including parametric, non-parametric and signal decomposition methods. The statistical power of these techniques as well as their suitability for identifying change is discussed. Using the uniquely detailed hydrochemical datasets generated under the Demonstration Test Catchments programme in England, the efficacy and robustness of change detection methods for hydrochemical data series is assessed. A conceptual framework for choosing a change detection method is proposed, based on this analysis, in order to raise awareness of the types of questions a researcher should consider in order to perform robust statistical analyses, for informing river catchment management and policy support decisions.

1. Introduction

Hydrochemical datasets are typically a product of many interacting variables and processes, which operate at a range of temporal and spatial scales. Markedly different behaviours can be evident in riverine hydrochemical datasets for a single catchment, relative to differing catchment hydrological responses to inter-annual climatic variability. At catchment scale there is a need to understand the effects of point source and diffuse pollution inputs as well as in-river transformations which drive both short- and longer-term trends within water quality. The introduction of the European Union Water Framework Directive (WFD – European Parliament, 2000) has increased the urgency of the need both to assess the current degree of water pollution and to examine the effectiveness of targeted mitigation options and strategies at catchment scale. It is therefore necessary to adopt suitable methods for detecting trends and change within hydrochemical datasets that are statistically fit for purpose.

One of the main challenges is distinguishing catchment responses that are due to deliberate manipulation associated with targeted intervention (e.g. on-farm) from those which are caused by natural variability in the catchment system. There have been numerous examples in the literature where the effects of mitigation strategies could not be resolved through the background environmental noise (Lord et al., 2002; Bechmann et al., 2005; Sohier and Degre, 2010). The mechanisms driving responses to mitigation observed in catchments have been shown to be difficult to pin-point due to incomplete knowledge regarding process controls on catchment nutrient cycling dynamics (Cirmo and McDonnell, 1997; Burt and Pinay, 2005) and ecosystem functional and structural responses (Band et al., 2001; Viglizzo et al., 2004; Cherry et al., 2008).

Given increasing efforts to implement mitigation in river catchments in order to comply with the EU WFD requirements it is critical to understand how much data, both in terms of record length

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and data resolution, is required to identify and correctly attribute these impacts to targeted mitigation alone. Research has shown, for instance, that in groundwater-dominated catchments, a large distribution of travel times exists due to variable depths of the water table, which can result in a range of residence times of pollutants (years to multiple decades) and significant lags between activities in the catchment and a response being seen in-stream (Smith, 1970; Headworth, 1972; Young, 1976; Wellings, 1984; Barraclough et al., 1994; Neal et al., 2004; Jackson et al., 2006; Howden et al., 2011). The design of representative sampling in terms of temporal resolution depends on the parameters or processes being measured and the scientific questions being addressed. Sampling often focuses on times of high-flow as storm events are well known to be an important driver of pollutant redistribution, both from land to water, and from remobilisation and flushing of accumulated in-channel stores and exchanges with the hyporheic zone. However, research has demonstrated that low flow conditions are also important since even drizzle can result in significant inputs of agricultural pollutants from impermeable surfaces such as farmyards, roofs and degraded road margins (Edwards et al., 2008; Collins et al., 2010). Given the need to capture the impact of pollutant mobilisation and delivery to rivers from less rainfall-dependent sources, there has been a move towards new high temporal resolution hydrochemical monitoring (Kirchner et al., 2004) for extending knowledge of catchment scale water quality behaviour.

The Demonstration Test Catchment (DTC) project, funded by the UK Department for Environment, Food and Rural Affairs (Defra) is currently monitoring hydrochemical and ecological responses to targeted on-farm mitigation. With the emphasis now placed on collecting longer and higher-resolution datasets in programmes such as DTC, it is necessary to make sure the potential of the new data rich records is fully exploited using the most appropriate methods of analysis, including an appreciation of the uncertainty associated with those analyses. This paper assesses change detection methods for hydrochemical data series in the context of the datasets being generated by the DTC programme.

A review of methods for detecting trends was produced by Esterby (1996), who considered both parametric and non-parametric methods for assessing monotonic trends in hydrological time-series. This was updated by Kundzewicz and Robson (2004), while Shumway et al. (2002) provide a more recent review of change detection in hydrological time series, but only consider traditional statistical approaches. As a result, there is a need for an updated, comprehensive assessment, taking into account the more complex visual and signal decomposition methods developed in recent years to analyse patterns within high-resolution hydrological and hydrochemical time-series. This paper first considers the challenges involved in the analysis of hydrochemical data time series and how these issues impact on the choice of analytical technique. It then considers the suitability and associated uncertainties of methods currently employed in hydrochemical research, and also considers methodologies used in other disciplines which may be applicable to analysing hydrochemical datasets.

2. The challenge of quantifying change due to mitigation

2.1. Uniqueness and uncertainty in catchment behaviour

There is a considerable challenge in quantifying changes to water quantity and quality in any catchment because of the underlying complexity of the system behaviour at that scale coupled with uncertainties and gaps in our techniques, observations, and conceptual understanding. (Environment Agency, 2011). Catchment hydrochemical behaviour is complex, combining a distribution of behaviours contributed by the different sources in the landscape, and the activation of different flow pathways linking these sources to the water body through variation in catchment hydrological function and human intervention (see Fig. 1). These produce concentration and load dynamics that vary significantly depending on rainfall events, which in turn, depend on the time of year and antecedent conditions. This is further complicated by human activities in the catchment which may generate pollutant fluxes which are not triggered by local climatic or hydrological behaviours and are not predictable with traditional hydrological modelling approaches. Examples would include the cutting of plant beds within rivers as part of a fisheries management plan, the accidental spillage of pollutants within the landscape particularly within farming operations, or river bank collapse through erosion of the substrate in prior extreme flow events, human intervention or livestock grazing in the river corridor. Within largely hydrologically-driven data sets, previous research has shown that trends in stream chemistry may be initially more apparent in high flows than low flows due to the interaction of different flow pathways (Murdoch and Shanley, 2006a). Much of the science that underpins the detailed understanding of these hydrological and biogeochemical pathways and transformations remains poorly understood (Beven and Alcock, 2012). Importantly, when detecting change driven by targeted mitigation in catchments which have historically undergone significant impacts (i.e. intensification of agriculture, structural land use change or water resource management and manipulation), we may not be able to justify the critical assumption of stationarity (Wagener et al., 2010; Khare et al., 2012). The extent and magnitude of the effects of these prior changes will be dependent on the historical context and timescale over which change has occurred, the residence times and distribution of travel times for flow pathways linking sources to the water body, the degree of accumulation of pollutant stores within the catchment, any underlying aquifer, and the stream channel itself, and process controls on the mobilisation and re-release of these materials under changing environmental conditions as mitigation is implemented. Past hydrological and hydrochemical behaviour may not always have an effective baseline against which changing behaviour through manipulation can be robustly assessed, especially where human interventions have significantly altered the baseline state. This should be reflected in the inferences made regarding any mitigation impacts, especially where changes are likely to be subtle, rather than extreme.

If it is assumed that every catchment is unique (Beven, 2000), then it must also be recognised that transferring knowledge and understanding from experimental and modelling approaches applied to relatively few catchments to identify best mitigation and management practice across large numbers of catchments with varied landscapes character and function requires a considerable amount of caution. The uncertainties in the evidence of change, within the context of those associated with capturing catchment attributes such as critical flow pathways, must be taken into account before this can realistically be used to underpin the development of catchment management plans more strategically. Nonetheless, it is impractical to monitor everywhere and on this basis, spatial extrapolation is inevitable, but dependent on the robustness of any statistical inferences made regarding the impacts of targeted pollutant mitigation.

2.2. Methodological challenges

There are a number of common problems relating to hydrochemical datasets which need to be considered when choosing a suitable method for detecting change or trends (see Fig. 1). The sampling strategy may significantly affect the methods that can be applied depending on sample irregularity and resolution.