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Considerations for integrative environmental assessments of contaminated estuarine sediments

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Abstract
Purpose – The purpose of this paper is to discuss integrative environmental assessments applicable to estuarine sediments, including the advantages and limitations of different lines of evidence that could form part of such assessments and their application to ecosystem services.
Design/methodology/approach – Weight of evident framework integrating multiple lines of evidence for sediment quality assessment.
Findings – Integrative environmental assessments are required to fully address the risks to resident fauna of anthropogenic contaminants deposited in estuarine sediments.
Originality/value – The paper presents an updated discussion of the methodologies for environmental assessments of contaminated estuarine sediments.
Keywords Seas, Rivers, Sedimentation, Contamination, Estuaries, Sediments, Environmental assessment, Toxicity, Weight of evidence, Risk assessment
Paper type Literature review

1. Introduction
Estuaries are highly productive yet complex ecosystems where anthropogenic contaminants can have potentially greater impacts than in marine ecosystems (Chapman and Wang, 2001; Elliott and Whitfield, 2011). However, early warning of such potential impacts or even determining where such impacts have occurred is more difficult in the transitional waters of estuaries than in truly marine or freshwater ecosystems.

Sediments figure extensively in the Millennium Ecosystem Assessment (2005) in terms of ecosystem services (see definitions in Section 2); however, contaminated sediment is not the dominant concern in that document. Rather, the focus is on land and water use and management on the landscape scale, which can profoundly affect sediment quality, quantity and fate. This focus includes the following, which can have significant consequences for biodiversity and the provision and resilience of ecosystem functions and services (Apitz, 2012): habitat change and loss due to changes in sediment inputs; changes in nutrient inputs with resulting changes to primary productivity; and, disturbance due to development and fishing practices. Contaminated

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sediments may not provide the ecosystem services of uncontaminated sediments, but they can certainly detract from those services and thus need to be adequately assessed and remediated, where necessary.

Contaminated sediments have gained prominent attention as a key component of integrative assessments due to the complex mixtures of chemicals that commonly characterize them (DelValls *et al.*, 1999). Estuarine sediments serve as a reservoir of contaminants, which can be mobilized as seasonal and other changes in physico-chemical cycles occur (Geesey *et al.*, 1984). Habitat variations within estuaries can provide resident fauna with more or less opportunity for exposure to such contaminants. Therefore, sediments act as an integrator and amplifier of the concentrations of anthropogenic chemicals in the waters which pass over and transport them. For this reason sediments have been widely used to identify sources of contamination, to measure the extent of such contamination, and to diagnose the environmental quality of aquatic systems (Luoma, 1990), including ecological risk assessments (Caeiro *et al.*, 2009).

In this paper we discuss methods and approaches to assess sediment contamination in estuaries, focussing on integrative (weight of evidence) environmental assessments. We outline the advantages and limitations of different lines of evidence that could form part of such assessments. We also discuss the implications of contaminated estuarine sediments to estuarine ecosystem services.

2. Estuaries are unique

Whitfield and Elliott (2012) define an estuary as "a semi enclosed coastal body of water which is connected to the sea either permanently or periodically, has a salinity that is different from that of the adjacent open ocean due to freshwater inputs, and includes a characteristic biota." Estuaries are physico-chemically more variable than other aquatic systems, but estuarine communities are less diverse taxonomically and the individuals are more physiologically adapted to environmental variability than equivalent organisms in other aquatic systems (Chapman and Wang, 2001). Further, estuaries are unique from other ecosystems in having "simultaneous connectivity to freshwater catchment and terrestrial influences, the atmosphere and marine systems" such that they are "multi-faceted ecosystems" (see Elliott and Whitfield (2011) for detailed discussion of other unique facets of estuaries). Estuaries show high spatial heterogeneity and complexity, a high fragmentation of habitats (Dauvin and Ruellet, 2009) and, because they are naturally stressed, it can be difficult to detect additional anthropogenic stress without focussing on ecosystem function rather than structure (i.e. on ecosystem services: Elliott and Quintino, 2007).

In addition to salinity gradients, estuaries also have strong gradients in other parameters, such as temperature, pH, dissolved oxygen, redox potential, and amount and composition of bedded and suspended sediments. However, salinity (overlying and interstitial), which varies spatially and temporally, is the major controlling factor for partitioning of contaminants between sediment and overlying or interstitial water. Salinity also controls the distribution and types of estuarine biota; for instance, benthic infauna are affected by interstitial salinities that can be very different than overlying salinities, resulting in large scale seasonal species shifts in salt wedge estuaries (Chapman and Wang, 2001).

The European Water Framework Directive (WFD) 2000/60/CE (European Commission (EC), 2000) requires member states to periodically monitor their estuaries and to achieve at least good water quality status by 2015. Article 8 of EC (2000) requires that member states establish programs for the monitoring of water status in order to establish "a coherent and comprehensive overview" of water status in each water body. Monitoring is required to establish the status of water bodies identified as being at risk of failing to achieve their environmental objectives. Monitoring programs are designed in accordance with WFD requirements and include monitoring of sediments and of the benthic environment, recognizing the unique and valuable role of estuaries in providing ecosystem services (Hartnett *et al.*, 2011).

3. Estuarine ecosystems services

Ecosystem services can be defined as the conditions and processes through which natural ecosystems, and the species they include, sustain and fulfill human life (Daily, 1997; Atkins *et al.*, 2011). They can also be defined (Fisher *et al.*, 2009) as "the aspects of ecosystems utilized (actively or passively) to produce human well-being." As noted by the Millennium Ecosystem Assessment (2005), human well-being is dependent upon the services provided by functioning ecosystems, which can be classified into four generic categories of services: provision, regulation, cultural and supporting. Beaumont *et al.* (2007) and Atkins *et al.* (2011) suggest that there are in fact five categories of services applicable to marine and estuarine ecosystems: production (e.g. food, transport, energy, human settlement); regulation (e.g. waste and climate regulation); cultural and spiritual, which are non-material (e.g. leisure and recreation, sense of place); supporting services, which are necessary but do not yield direct benefits to humans (e.g. habitats for food species and the prey they depend upon); and, option use values, which are associated with safeguarding the option to use the ecosystem in an uncertain future.

Estuaries are highly fertile areas and their associated terrestrial environments are the focus of large human settlements because of that fertility and other services they provide. However, because of their desirability estuaries are also subject to a variety of anthropogenic stressors ranging from habitat loss and introduced (e.g. aquaculture)/invasive species (e.g. from ballast water) to contaminant inputs, arguably more than for any other aquatic system (Elliott and Whitfield, 2011). Contaminant inputs tend to accumulate in estuarine sediments which, as previously noted, can be both a sink and a source for contaminants that can have adverse effects on biota and thus on estuarine ecosystem services. Identification of past, present or potential future risks associated with contaminated sediments is critical to the preservation of estuarine ecosystem services (Pinto *et al.*, 2010).

As suggested by Schäfer *et al.* (2012), the first step for ecological risk assessment (or a weight of evidence assessment) based on ecosystem services is to identify the relevant ecosystem services for a specific environmental compartment, in this case bedded sediments, then to derive suitable measurement endpoints. In other words, ecosystem services comprise the assessment endpoints that are to be protected, linked to the ecological risk assessment or weight of evidence assessment by ecological models (Galic *et al.*, 2012). A full, detailed list of all ecosystem services provided by estuaries has not, to our knowledge, been provided. We would expect such a list to be similar to that developed by Harrison *et al.* (2010), for freshwater ecosystems. However, we caution that investigators should not be restricted in their assessments by the obvious (i.e. to focussing only on aquatic species), given the previously noted multi-faceted nature of estuaries. For instance, contaminated estuarine sediments can pose a risk to wading birds (Smith *et al.*, 2009). Pastorok and Preziosi (2011) propose a framework for assessment of ecosystem services that builds upon quantitative analysis of ecological structure-function relationships.

4. Assessment of sediment quality

Various lines of evidence are available for the assessment of sediment quality (Chapman and Hollert, 2006) as are various methods to integrate those lines of evidence. Such integration involves either hazard (possibility) or risk (probability) assessment (Shin and Fong, 1999; Smith *et al.*, 2002; Grapentine *et al.*, 2002; Benedetti *et al.*, 2012).

There is no consensus on a single process to integrate multiple lines of evidence, nor does there need to be, so long as the integration is transparent and involves at a minimum both chemical measurements of exposure and biological analyses of effect. Such integration is typically called a weight of evidence evaluation (Wenning *et al.*, 2005). Weight of evidence methods typically comprise the screening level of an ecological risk assessment (Chapman and Anderson, 2005; Chapman, 2007a).

The first sediment weight of evidence proposed was the Sediment Quality Triad (Long and Chapman, 1985; Chapman 1990, 1996; Chapman *et al.*, 1987, 1997), which still forms the foundation for most sediment weight of evidence assessments and evaluations. Such assessments can assist in determining when chemical contamination (the presence of a chemical above background or reference levels) becomes pollution (contamination that causes adverse biological effects), its ecological significance (e.g. are populations or communities of organisms at risk, not just individual organisms?), optimal remedial options and the urgency of corrective actions (Burton *et al.*, 2002).

The Sediment Quality Triad incorporates three essential components or lines of evidence (DelValls *et al.*, 1999; Chapman and Hollert, 2006): measures to determine the presence and degree of anthropogenic contamination; measures to demonstrate that substances that are present can interfere with the normal functioning of at least some biological organisms tested in the laboratory; and, assessment of the status of resident biological communities (e.g. is there alteration relative to reference conditions?). Additional components are causation, which can be assisted by the use of biomarkers (Morales-Caselles *et al.*, 2009), and ecological relevance (Morales-Caselles *et al.*, 2008).

The presence and degree of anthropogenic contamination is typically assessed by comparisons to background or reference conditions and/or the use of numeric sediment quality benchmarks (SQBs). Examples of the latter include the "threshold effect level/ probable effect level" (MacDonald *et al.*, 1996) and the "effects range low/effects range median" (Long *et al.*, 1995). However, SQBs need to be used with care since they tend to be highly conservative as they are based on total chemical concentrations without consideration of bioavailability or of contaminant/other stressor/modifying factor interactions, and thus are not alone sufficient for management decision making (Wenning *et al.*, 2005). Further, they tend to be generic rather than site specific. There have been few attempts to develop site-specific SQBs (e.g. DelValls and Chapman, 1998; Choueri *et al.*, 2009).

Information on the bioavailability of sediment contaminants can be provided by bioassays, either bioaccumulation or toxicity tests. Bioaccumulation is a phenomenon, not an effect; however, the fact that organisms can accumulate contaminants does indicate that they are bioavailable although it does not indicate that those contaminants can or will cause adverse organism-level effects (Landrum *et al.*, 2011). Laboratory toxicity tests can provide for rapid and cost-effective screening of contaminated sediments (i.e. are sensitive laboratory surrogates harmed by exposure to those sediments?). The use of sediment chemistry, bioaccumulation and toxicity testing can be effective in determining sediments and contaminants of potential concern (Beiras *et al.*, 2003).

Toxicity test organisms need to be appropriate to the problem being addressed, and the results put into context relative to reference and/or baseline comparisons to understand hazard. However note that, with global climate change, comparisons to baseline will in future no longer be possible (Chapman, 2011a), thus future comparisons must be to reference conditions which are naturally highly variable in estuaries (Barbone *et al.*, 2012). Note also that truly estuarine species are relatively few compared to freshwater or marine species and thus the possible pool of test organisms is also relatively small (Chapman and Wang, 2001). Typically sediments are sieved prior to toxicity testing to remove the possibility of biologic interference by resident organisms, however, sieving will result in changes to sediment chemistry, which need to be taken into account when evaluating this line of evidence (Fisher *et al.*, 2004). Also, toxicity test endpoints need to be appropriate (i.e. ideally include survival, growth and fecundity so that individual organism responses can be extrapolated to populations and communities), while recognizing that statistical significance is not equivalent to ecological significance, and transparently documenting uncertainty (Chapman *et al.*, 2002a).

Toxicity testing is commonly conducted in the laboratory, but it can also be conducted in the field (i.e. *in situ*). For instance, caged animals have been used to measure biomarkers, bioavailability (chemical residues), histopathology and even mortality (Martın-Dıaz *et al.*, 2004; Morales-Caselles *et al.*, 2009; Costa *et al.*, 2011a, 2012). The combination of conservative laboratory and more realistic field testing can be particularly useful for weight of evidence determinations and for ecological risk assessment (Morales-Caselles *et al.*, 2008). However, because of cost considerations, less expensive laboratory tests are typically used for screening and for determining how and where to apply more expensive field tests (Costa *et al.*, 2011b). Field testing typically comprises the detailed level of an ecological risk assessment while laboratory testing would comprise the initial screening level (Chapman and Anderson, 2005).

Biomarkers also have a role in weight of evidence assessments and in ecological risk assessment (Riba *et al.*, 2004; Chapman and Hollert, 2006; Benedetti *et al.*, 2012). For instance, Costa *et al.* (2008, 2009, 2011a, b, 2012) assessed both cellular toxicity mechanisms and contaminant bioavailability using estuarine benthic fish exposed to contaminated sediments in laboratory and *in situ* bioassays. While most biomarkers measure exposure, some biomarkers measure effects – both types can provide early warning of potential meaningful ecological effects in combination with other lines of evidence (Martın-Dıaz *et al.*, 2004). Biomarkers can also be used to determine cause-and-effect, linking the bioavailability of chemicals with their concentrations at target organs and intrinsic toxicity. However, as with all lines of evidence, biomarkers need to be used with care and with knowledge of what information is and is not provided. For example, while some biomarkers are specific to certain groups of chemicals, others are less specific. Further, biomarkers of exposure should not be confused with biomarkers of effects. Finally, presumably because of their relatively high sensitivity, biomarker responses can sometimes be difficult to interpret (e.g. these may be false positive responses).

Benthic community field surveys were and remain part of the Sediment Quality Triad and provide critically important ecologically relevant information (Chapman *et al.*, 2002b). The condition of the ambient benthic community can serve as a reliable and sensitive indicator of potential disturbances resulting from chemical stressors (Hyland *et al.*, 2003) or from natural conditions (Casazza *et al.*, 2002). Without benthic community data, decisions cannot always be made as to whether the sediments are polluted as opposed to contaminated (Chapman, 2007a, b). However, the main disadvantage with this line of evidence is the natural variability of benthic communities, particularly in estuaries where alteration is more common than stability (Chapman and Wang, 2001). Another disadvantage is that such surveys provide no information on potential tolerance of resident communities to chemical pollution, either through physiological acclimation or genetic adaptation, or of the energy requirements of such tolerance that could affect critical population-level parameters such as reproduction (Chapman, 2007b). Tolerance can also take the form of lifestyle changes, i.e. avoidance of contact with toxic sediments (Rubal *et al.*, 2011), again with energetic costs.

5. Integrative environmental assessments

Integrative (i.e. weight of evidence) assessments are science based. However, as such they form only one component of management decision making, which also must factor in, for instance, social or economic factors (Linkov *et al.*, 2009; Caeiro *et al.*, 2009).

As noted above, single lines of evidence can be used for screening but multiple lines of evidence are required for a weight of evidence assessment (Chapman *et al.*, 2002b). Initially summary indices had been suggested for use in Sediment Quality Triad weight of evidence assessments (Chapman *et al.*, 1987). However, such indices, because they compress information and can easily be misunderstood by non-scientists, are no longer recommended for these and other reasons provided in Chapman (1996), Chapman *et al.* (2002b), Green and Chapman (2011) and Chapman (2011b). Unfortunately, indices continue to be used because single number values have appeal to both scientists and non-scientists (Schmidt *et al.*, 2002; Lee *et al.*, 2006; Piva *et al.*, 2011; Benedetti *et al.*, 2012).

There are currently two different, valid means to assess the individual Sediment Quality Triad lines of evidence in a weight of evidence evaluation, which are not mutually exclusive: multivariate analyses and/or tabular decision matrices. Appropriate reference comparisons are desirable (Chapman, 1996) but not always essential. Appropriate application design and application of factor analysis (Riba *et al.*, 2004; Morales-Caselles *et al.*, 2008, 2009; Caeiro *et al.*, 2009; Costa *et al.*, 2012) does not require reference stations or comparisons.

Multivariate analyses are gaining in popularity (Shin and Fong, 1999; Beiras *et al.*, 2003; Riba *et al.*, 2004; Zhang *et al.*, 2007; Cesar *et al.*, 2007; Benedetti *et al.*, 2012). Such analyses can involve, but are not restricted to: principal component analysis (e.g. Chapman, 1996; Anderson *et al.*, 1998; Morales-Caselles *et al.*, 2009; Caeiro *et al.*, 2009); cluster analysis (e.g. Shin and Fong, 1999); non-metric multidimensional scaling (e.g. DelValls *et al.*, 1998; Beiras *et al.*, 2003); discriminant analysis (e.g. Shin and Fong, 1999); correspondence analysis (e.g. Rakocinski *et al.*, 1997); and BIO-ENV procedure (e.g. Mucha *et al.*, 2003). Software tools to integrate statistical data for integrated sediment quality assessment have also been developed (e.g. Khosrovyan *et al.*, 2010).

Tabular decision matrices were originally proposed by Chapman (1990), and are based on hit/no hit alternatives formatted for decision making. A primary limitation of this approach is that it does not explicitly incorporate variance into the quality of the different lines of evidence. It is assumed that the data from each line of evidence component are appropriate. The hit alternatives are therefore classified according to a logic system that weights the strength of evidence that supports each potential outcome (Burton *et al.*, 2002; Chapman *et al.*, 2002b), and which can be summarized as follows: the adverse effect must be associated (e.g. correlation, which is not causation) with exposure to the stressor; the stressor must be found in the affected receptor (i.e. must be bioavailable); the adverse effect must be manifest in unimpaired species under controlled experimental conditions (e.g. in the laboratory); and, the adverse effect must be found in the affected species (i.e. in the field). These alternatives and in fact the tabular decision matrix can be and in fact often are based on multivariate analyses (Chapman, 1996; Caeiro *et al.*, 2009).

Determination of causation follows the weight of evidence assessment (Chapman and Anderson, 2005) and must establish a relationship that is more than correlative between the suspect chemical(s) and the adverse effect(s) (Rand, 2008). Some of the lines of evidence used in the weight of evidence assessment can assist in this determination; however, the exact lines of evidence used will depend on the outcome of the weight of evidence and on best professional judgment, which comprises the use of expert opinion and judgment based on available data and site- and situation-specific conditions.

Best professional judgment also plays a role in weight of evidence assessments. For example, Albertelli *et al.* (2003) applied a Sediment Quality Triad incorporating best professional judgment. The weight of the different components was computed based on expert judgment according to the Delphi method (Weaver, 1971) with the results of each line of evidence calculated using the dashboard free software (Processdash, 2004). Piva *et al.* (2011) also used best professional judgment in their weight of evidence contaminated sediment assessment. Elliott and McLusky (2002) suggest that best professional judgment is essential for estuarine assessments given the complexity of these ecosystems.

Best professional judgment can be initiated when there are extensive data but few uncertainties as well as when there are few data and many uncertainties; however, the former is likely to provide the most defensible results. The use of best professional judgment was evaluated by Bay *et al.* (2007) for the Sediment Quality Triad and by Thompson *et al.* (2012) for the benthic community line of evidence. High levels of agreement were not the norm between experts. In fact, Thompson *et al.* (2012) noted that the lack of agreement under estuarine conditions makes agreement regarding pollution status problematic. Greater levels of agreement are obtained when there is a clear conceptual model, there is clarity regarding protection goals (i.e. ecosystem services), and the investigation and the study objectives are aligned (Chapman, 2007a).

The use of best professional judgment in weight of evidence assessments results in uncertainty, but this is not the only source of uncertainty in such assessments. Uncertainties in weight of evidence assessments are discussed by Burton *et al.* (2002) and Chapman and Anderson (2005) and need to be explicitly discussed as they are in an ecological risk assessment, such that management and other non-scientific decisions can be made with full cognizance of remaining uncertainties and their potential significance. Explicit discussion of uncertainties needs to include, but not be restricted to:

- development of a conceptual model during problem formulation that is based on ecosystem services and which recognizes the unique nature of estuaries;

- linkages between chemicals of potential concern and receptors within the broader context of ecosystem services and estuarine variability;
- identification of other natural and anthropogenic stressors with associated exposure dynamics;
- determination of appropriate reference comparisons;
- consideration of the advantages and limitations of different lines of evidence and of the quantification methods used to integrate them into a weight of evidence assessment; and
- evaluation of causality and level of environmental concern/significance.

6. Conclusion

Weight of evidence methodologies have been widely used including within ecological risk assessment, although the choice of line of evidence and of integration methods cannot be depicted in "cook book" format, in other words, cannot be prescribed. There is as much art (i.e. best professional judgment) as science in the use of weight of evidence for contaminated sediment assessments because of the site- and situation-specific nature of such assessments, which is amplified in estuaries compared to fresh and marine water bodies. This paper provides information that we hope will be of assistance to both those familiar with and those unfamiliar with contaminated sediment assessments and with weight of evidence for such assessments in estuaries within the context of ecosystem services.

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