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# Weight-Of-Evidence-based Assessment of Sediment Quality of the São Francisco River (Brazil) with the Help of Software Tool SQA

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**Abstract:** Weight-of-evidence (WOE) approach is a requirement for comprehensive integrated sediment quality assessment and management worldwide. WOE is a system approach based on collection of several lines of evidences that are able to derive multi-aspect characterization of availability and adverse effects of contaminants for living organisms in water environments. A software tool addressing this approach is already available and based on the statistical package STATISTICA 6.0. The tool provided user-friendly and user-assisting interface for entering and analyzing of data, as well as presented a summary of the results of the conducted analysis. It was designed for environmental scientists and managers, academia and all those who are interested in integrated sediment quality assessment. The present work is the new version of the software based on another statistical package - SPSS 11. This increases usability of the tool for different users. The present work also demonstrates a case study: WOE approach used in sediment quality assessment for River São Francisco, Brazil. Holistic analysis of sediment contamination status along the riverside was performed by integrating different lines of evidences collected at different contaminant loads in the environment. The outcome of this analysis is a summary of the harmful effects caused by contaminants at different studied sections. The results can be used by environmental managers and decision makers for selecting best management option for reducing contamination level in the sediment and preserving healthy status of the river.

*Keywords:* Software tool; weight-of-evidence; toxicity; model.

## 1. INTRODUCTION

The weight-of-evidence (WOE) philosophy, as commonly applied in sediment quality assessment, has already proved its consistency and robustness by e.g., Borgmann et al. [2001], Chapman et al. [2002], Chapman [2007].

Multiple lines of evidence from different dimensions (sediment chemistry, lab toxicity, in-situ observations) and interpretation of causality between them form the basis of the philosophy. For example, sediment physical properties are interpreted in terms of their influence on contaminant availability and biological responses. As it was already shown by Carpentier et al. [2002], fine sediment adsorbs more organic matter and metals compared to coarse ones.

Many integrative methodologies forming the WOE framework have already been created and successfully applied as shown in the works of Casado-Martinez et al. [2007], DelValls and Conradi [2000], Riba et al. [2006]. However, new lines of evidence are constantly developed e.g. by Brack et al. [2005], Chapman and Hollert [2006], Martin-Diaz et al. [2004], spanning different exposure pathways, species and responses (biological activity inhibitions, biomarkers). Hence, the methodologies may vary from an investigation or a research group to the other.

A variety of software tools ranging from decision-support systems to sophisticated models is available nowadays for addressing different research and management needs. Some examples include works by Fisher et al. [2012], Khosrovyan et al. [2010], Panagopoulos et al. [2012]. The presented software tool is designed for assessing sediment quality in aquatic environment by 3 different WOE methodologies. The methodologies can be used as separately so in combination depending on the desired dimension of the assessment. When combined, they provide multi-aspect evaluation of sediment quality.


## 2.    METHODOLOGY


### 2.1    Weight-Of-Evidence Framework Methodology Used in the Software Development

SQA is the computer program, which provides tools for applying three weight-of-evidence methodologies. The WOE methodology groups similar variables into a corresponding domain. Thus, the environmental contamination domain spans sediment chemical concentration (metals, organics) and physical parameters (grain size, organic carbon content); the toxicity domain refers to toxicological responses obtained by laboratory testing; the alteration domain may include benthic community structure changes or toxicological responses obtained in-situ. There are totally three domains, which represent a triad.

The data from various domains are integrated via different analytical tools. This allows interpretation of the results by uncovering causal links between them. Such integration is known to provide a solid base for assessing ecological relevance of the observed pollution (pollutant bioavailability, compartmentalization, induced effects). In some cases, deficiency in data might be indicated as well, for example, the evidence from measured data may not be supported by that obtained in-situ.


### 2.2    Software Description

The program consists of three blocks, each representing the separate WOE methodology based on: 1) sediment quality triads, 2) statistical multivariate analysis (principal component analysis) and 3) statistical one-way ANOVA Dunnett test of statistically significant differences.

The results of the first block represent triads (triangles) which vertices demonstrate pollution indexes calculated for each of the domains. The triads are compared with the reference triangle corresponding to a contamination-free or contamination-low state. The comparison allows understanding of the bioavailability of the contaminants, their effects on aquatic organisms (toxicity tests) and ecological malfunctioning (benthic community changes). The program's output is a graphical representation of the triads.

The second block interprets causality between sediment contamination and biological effects by means of the principal component analysis (PCA). The results are interpreted to identify the pollutants that caused the observed biological effects and the locations where these effects were critical. The output consists of two tables: component loadings and scores.

The last block analyzes pair-wise statistically significant differences between pollution indexes calculated for the reference and the sample sites by means of the one-way ANOVA Dunnett test. The output of the program consists of colored diagrams in the form of pie-charts, corresponding to different confidence levels.

In addition to the characteristic output produced by each block, the program also provides a textual interpretation of the results. This facilitates reading of the statistical and graphical outputs for a general user. The output can be saved in the program installation path.

During each execution step, the program provides informative and short guidance to the user. In case of erroneous situation (e.g., missing file) the program provides explanative prompts and in case of irrecoverable errors, stops execution.

The program is developed in Java 1.5 programming language for PC computers. The program has been tested in WinXP and Win7 Starter and Home Premium OSs. The statistical analysis is performed by means of SPSS11.

The reliability of the program was checked by comparing the program's output with the manually obtained one. The comparison demonstrated identical results.

The program was first released in 2011 in English version. Program size is around 500 KB excluding size of SPSS11 package. The tool is distributed as a package with the executable and SPSS macro and script templates.

The program development pursued the objective of offering the full functionality for conducting integrated sediment quality analysis through a simple-to-use computer program. The overall process of the integrated analysis is time-consuming and requires certain scientific background. The tool addressed this issue by facilitating the whole process with respect to time, quantity and variety of data operations and analysis as well as interpretation of the results. The tool is equally useful for both professional users and those who lack specialized knowledge but need a science-based environmental quality assessment (environmental managers, monitoring agencies).

## 3.    STUDY AREA

A case study on the assessment of sediment quality in the upper-middle region of River São Francisco (Figure 1) is provided to demonstrate the software use, functionality and applicability for such assessment.

This water body is one of the most important Brazilian rivers, connecting the southeast and northeast regions of the country, representing a huge diversity of climates and biomes. The mentioned region of the river is affected by anoxic water entering from Três Marias reservoir, zinc-refining factory and human activity such as sewage effluents from the Barreiro Grande stream and other diffuse sources.

Sediment samples were collected by a Petersen grab of 5 liters capacity from 7 cm of depth at 9 sampling points located within Três Marias reservoir and the confluence with River Abaeté (SF-1, SF-2, SF-3, SF-5, SF-6, SF-7, SF-8, BG-4, ZM-2) (Figure 1). The samples were homogenized and stored in the dark at 4ºC for no longer than 15 days prior to the analysis. Samples for benthic analysis were collected separately; benthic animals were retrieved with the help of a 0.25 mm sieve and fixed in 40% formalin.

According to the WOE approach, the following LOEs were studied:

1) For the contamination domain: grain size distribution, total organic carbon content, concentration of 12 metals (Al, As, Ba, Cd, Co, Cu, Fe, Hg, Mn, Ni, Pb, Zn).

Determination of the metal concentration in the sediment was done according to the USEPA 3050B Method, adapted by García-Rico et al. [2006] and Trefry et al. [2002].

2) For lab toxicity domain: toxicological tests and biomarkers.

The toxicological tests were performed using different species: zooplankton *Daphnia similis* (ABNT [2004]), amphipod *Hyalella azteca* (ABNT [2007]), fly *Chironomus xanthus* (Fonseca and Rocha [2004]), lugworm *Branchiura sowerbii* (Arate et al. [2004]), fish *Prochylodus affinis* (for histopathological damages) and bivalve *Anodontites trapesialis* (for determination of neutral red retention time).
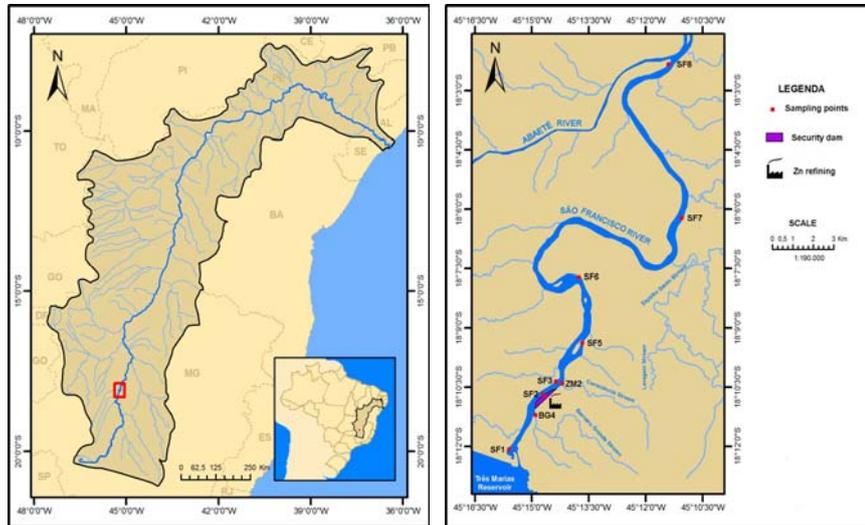


**Figure 1.** River São Francisco (Brazil): study area and sampling points.

In the acute toxicity tests, immobility of *D.similis* (48h day of exposure), survival *H. azteca* (10 days of exposure), *C.xanthus* larvae emergence (15 days of exposure), reproduction count of *B.sowerbii* (28 days of exposure) were checked. In the biomarkers tests, neutral red color by *A.trapesialis* and histopathological alterations in liver and gills of *P.affinis* after 28 days of exposure were measured.

3) For in-situ alteration domain: biological monitoring working party index (BMWP), measuring species tolerance to pollutants, and classical diversity index (Shannon index), determining species proportion.

The indexes were measured on family and class levels (families of Chironomidae, Tabanidae, Elmidae, Polycentropodidae, classes Gastropoda, Bivalvia, Oligochaeta, etc.)

As a reference point, SF1 was used. Due to its location before the Zn-refinery, the impacts from two important pollution sources (sewer and refinery) are excluded.

## 4. MODEL SET UP

The program interacts with an intended user through a series of simple and guided graphical user interfaces. At the start, the program provides options for selecting the methodology (Figure 2).

If the SQT-based methodology is selected, the program opens a new screen with two data processing options (manual or automatic). In case of manual processing, the program provides an interface for performing mathematical calculations (Figure 3). With the automatic data processing, the pre-defined set of mathematical operations (for data normalization) is automatically performed.

When finished, the program draws the triads, without any intervention by the user (Figure 4).

If the PCA-based option is selected, the user is prompted to indicate number of the components to be extracted and a threshold value for the component loadings (Figure 5). The analysis is performed with a little help by the user, namely by pressing a macro button on SPSS tool's panel.

ANOVA-based methodology is not demonstrated in this study and therefore not discussed.

In case of a missing domain data, it is recommended to apply PCA-based methods, as otherwise, the results might not be representative. For example, the triads will lack a lateral.
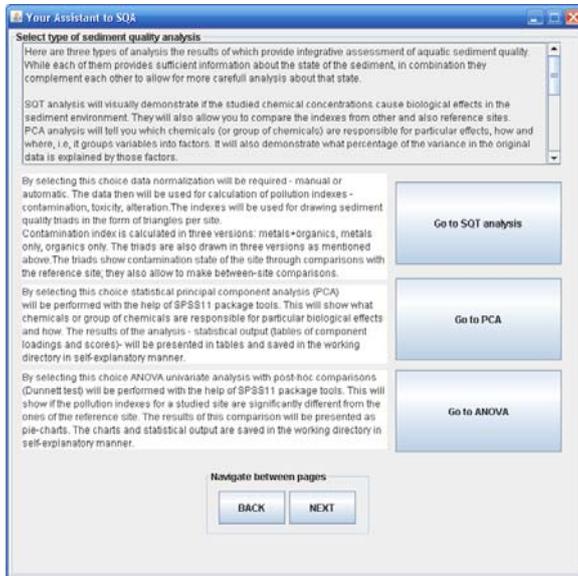
**Figure 2.** Panel for selecting integrated sediment quality assessment method.
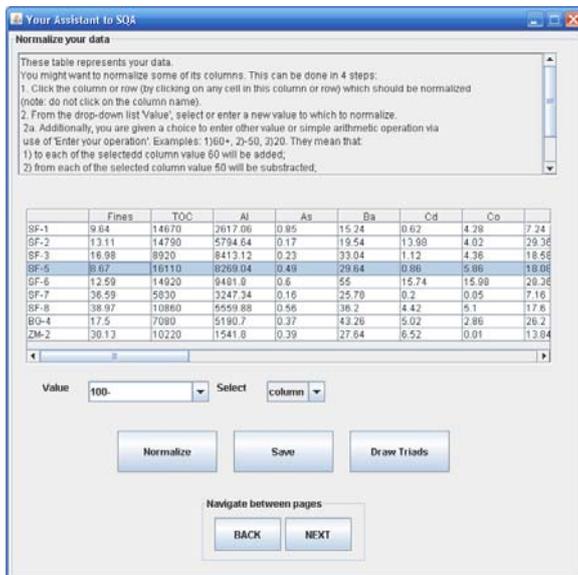
**Figure 3.** Area for mathematical data processing.

## 5.    RESULTS AND DISCUSSION

The results of SQT-based methodology showed that for many sites (BG-4, SF-5, SF-6, SF-8, ZM-2) elevated levels of metals were toxic to the animals exposed in the lab. The triads corresponding to those sites are similar to that shown on the left-side of the Figure 4. It can be seen however, that they did not affect the diversity of species and the tolerance to pollutants (no changes in the alteration domain). On one hand, the studied species might have developed tolerances to pollutions through adaptation to chronically high levels of chemicals.
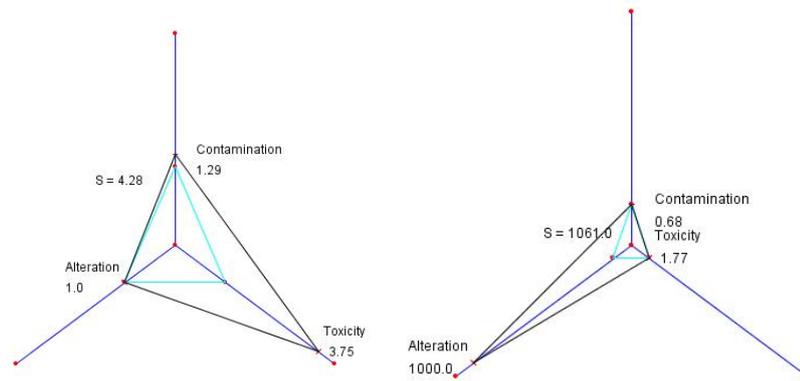
**Figure 4.** Sediment quality triads showing interactions of different domains. Light-blue triad shows pollution indexes of the reference site, dark-blue – those of the sample site. From left to right: contaminant stress and high toxicity in lab conditions; alteration in the benthic community and lab toxicity without contamination.
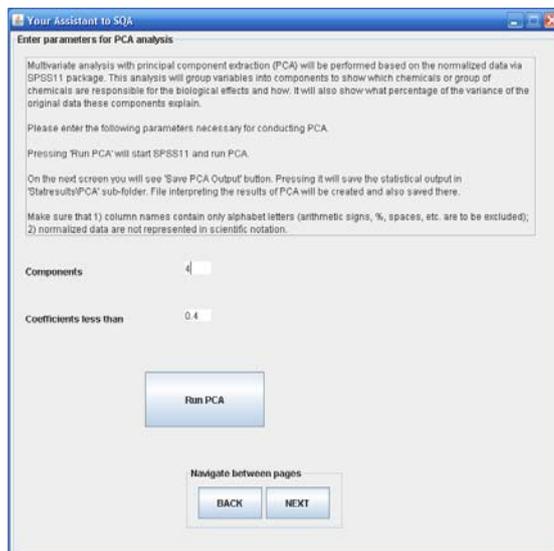


**Figure 5.** Parameters required for conducting principal component analysis: number of components and threshold value above which loadings are retained.

On the other hand, absence of ecological malfunctioning could mean that there might be other ecosystem-level effects, which were not addressed by this study (e.g. species abundance).

The sites SF-2, SF-3 and SF-7 have shown triads similar to those depicted on the right-side of the Figure 4. The alteration indexes considerably exceeded that of the reference site (dark-blue vs light-blue triads). High alteration and comparatively lower toxicity under the absence of contamination may be caused by other pollution sources not measured in this study (e.g., by influx of oxygen-depleted water or a sewer discharge).

For the PCA-based methodology, three components were extracted and component loadings ≥ 0.4 (by absolute value) were retained. The component #1 linked metal contamination to the laboratory toxicity (reproduction of lugworm). This component was predominant and accounted for 28% of the variance in original data.

The component #2 also related contamination with laboratory toxicity only (4 responses). This association was critical for the sites SF-2, ZM-2, BG-4 and SF-6.

The first three sites are located closely to the refinery and their sediment might have accumulated by-products from the refinery (Al, Fe, Cd and Pb waste) over the time along with other metals. Site SF-6 is quite far from the refinery, but it lies in a zone where water flow is slowed, according to Hidromares and IIE [2008, 2009]. This might contribute to the retention of contaminants in the sediment matrix rendering it toxic. This component accounted for 25% of the variance.

The last, third component (18% of variance) related the lab toxicity (3 toxicity responses) with in-situ alteration (2 responses). The relation was relevant to the sites SF-2, SF-3, SF-5 and SF-7. Sites SF-3 and SF-5 are characterized by fast currents due to hydrodynamic characteristics of the river as demonstrated by Hidromares and IIE [2009]. The alteration in these sites (tolerance and diversity of benthic animals) might be caused by fast currents that physically disturb the benthic community. Alternatively, other toxicants may enter from the disturbed sediments in bio-available form affecting the organisms.

Absence of in-situ changes (the components #1 and #2) might suggest that 1) there could be other types of ecological malfunctioning not considered presently and 2) diversity and tolerance indexes applied on family or class level may not be used as such for examining benthic population changes. Besides, the species used might not be bio-indicators of water pollution in the given areas, due to e.g., adaptation to high background chemical levels.

Absence of contaminants when toxicity and alteration are present (the component #3) suggests that there might exist alternative factors (other pollution sources) that were not taken into consideration. Sewage effluents flow through the sites SF-2, SF-3 and SF-7 and their effect on the benthic community should be analyzed as well.

Both methodologies (SQT- and PCA-based) indentified the same factors and interactions between them. Thus, in the sites BG-4, SF-6 and ZM-2, contamination was related to the laboratory toxicity only without in-situ alteration; in the sites SF-2, SF-3 and SF-7 in-situ alteration and laboratory toxicity were identified.

## 6.    CONCLUSIONS

The conducted preliminary research did not identify changes of diversity and tolerance of the benthos that could be provoked by metal contamination. This suggests that the metals are not bio-available in-situ. However, it urges to conduct a more detailed research that will account for as many potential pollution sources as possible (e.g., sewage or anoxia factor). Further research may uncover site-specific bio-indicator species of water pollution, which can be confidently used for examination of changes in benthic communities.

This study suggests that in-situ indexes should be calculated on individual level instead of family or class levels. Additionally, other parameters of benthic community structure can be employed (apart from BMWP and Shannon indexes).

SQT- and PCA-based WOE methodologies can be used independently as well as interchangeably and can serve many purposes: eco-toxicological, bio-monitoring, environmental management, decision-making.

The newly developed software SQA facilitates the processes of preparation, analysis and interpretation of integrated data in a fast, error-free, state-of-the-art and reliable manner. Built on the WOE methodologies and being a robust software tool with a few and simple user interfaces, SQA fosters better information management to the benefit of many interested stakeholders such as environmental scientists, educators, managers, monitoring specialists, eco-toxicologists.

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