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Development of an estuarine quality index based on key physical and biogeochemical features

J.G. Ferreira*

IMAR — Institute of Marine Research, DCEA-FCT, Qta Torre, 2825 Monte de Caparica, Portugal

Abstract

An index (EQUATION — Estuarine QUAlity and condiTION) is presented for integrated evaluation of estuarine quality, based on an aggregation of four different components: vulnerability, measuring the physical capacity of the system to react to change, water quality, which examines trophic status and eutrophication aspects, sediment quality, which looks at the sediments and benthic fauna, and trophodynamics, which addresses the quality and value of the top levels of the trophic web. The data requirements are reduced by the application of models and heuristic grading, and the four components are combined into a 1 (worse) to 5 (better) overall grade. The index was implemented as a decision support system, and it was tested on five different estuaries in the US and Europe. The test ecosystems were chosen to study a range of physiography, tidal regimes, organic loading and contamination by persistent pollutants. Scores ranged fom Low (grade 2) for the Elbe estuary to Excellent (grade 5) for Tomales Bay in California. Tests were also carried out on "concept" estuaries and using different scenarios for two of the chosen estuaries. The classification obtained is in agreement with other authors, and the methodology provides a useful synthesis of the basic descriptors of estuarine quality: physical aspects, water quality, benthos and higher trophic levels (including socio-economic aspects of fisheries). © 2000 Elsevier Science Ltd. All rights reserved.

1. Introduction

Classification and ranking systems for water bodies have been applied for many years, and are based on a wide range of different aspects, such as geomorphology and mixing characteristics [1,2], hydrology [3], or biotic features.

E-mail address: jgferreira@compuserve.com (J.G. Ferreira).

^{*} Tel.: + 351-21-2948300; fax: + 351-21-2948554.

Apart from this type of classification, concerns regarding water quality (sensu lato) have led to the development of other indices, aiming to categorise water masses from the standpoint of pollution, in order to assist management. These indices are usually based on three approaches:

- (i) The definition of classes corresponding to concentration ranges for indicator parameters such as dissolved nutrients.
- (ii) The use of synthetic approaches such as the saprobic index which use faunal diversity or some other indicator as a representation of the quality of the sediment and water column.
- (iii) Composite approaches linking several indicator parameters, such as sediment contamination and species composition.

The different types of indices which have been developed usually focus on a particular ecosystem compartment, and do not directly consider the different features of the environment as a whole. Historically, the development of these classification systems occurred in freshwater: examples of these indices are BMWP and ASPT [4,5] and IFIM [6,7]. These were applied for the comparison of different water bodies and for management, for instance regarding remedial measures. Some of these have been developed into decision-support systems (DSS), such as PHABSIM [8] or RIVPACS [9].

In coastal marine systems, environmental quality has been categorised using sediment quality metrics such as the sediment quality triad [10–12] or sediment quality guidelines [13,14], benthic indices such as the infaunal trophic index (ITI) [15], B-IBI [16] and water-column-based approaches such as TRIX [17]. Estuaries pose a particular problem in terms of classification from a quality standpoint, because features such as the tidal regime, flushing time or vertical stratification cause very different conditions to occur in the water column and sediment, and therefore a comparison of benthic infauna, or turbidity, or trophic status of different systems is not necessarily a good approach to analysing anthropogenic impact. Estuarine indices have been developed based on the benthic ecology [18], or on trophic interactions [19]. These approaches allow a detailed classification scheme to be implemented, but may limit the application of the indices to similar estuaries (e.g. Gulf Coast estuaries discussed by Engle et al. [18]).

The approach followed by Cooper et al. [20] is more fully integrated, using a three-part classification of estuarine quality (or condition), based on water quality, biology and aesthetics, supported by a physical basis. The methodology was tested using a series of estuaries in Natal (RSA) and is more management oriented than previous work, in that it has a higher built-in level of intercomparability between different systems. However, due to the fact that physical comparisons are only carried out at the geomorphological level, the approach is robust only for a regional dataset. Like all the approaches referred, it has a fairly large data requirement, which in estuaries is a particular concern, because of the temporal and spatial variability in these ecosystems.

There is a clear need for a more comprehensive approach to estuarine environmental quality classification, which takes into account physics, chemistry and biology on the one hand, and the water column and sediment aspects on the other. This is particularly important for the practical implementation of legislation which applies to large heterogeneous areas (e.g. the new European Union Water Quality Directive).

The challenges for such an approach are the data requirement and cost, and the difficulty in unifying the different components of such an index, allowing it to be comprehensive and yet of practical application.

In this paper, the development of an integrated estuarine quality and condition index (EQUATION — Estuarine QUAlity and condiTION) is outlined. The objective of the EQUATION index is to provide a simple final grade of estuarine quality and condition, on a scale of 1 (worse) to 5 (better), based on a combination of four different components. These are system vulnerability, measured on the basis of physical characteristics; water quality, based on nutrients, primary production and dissolved oxygen; a composite index of benthic quality; and an index of quality for higher trophic levels.

A decision support system has been developed, integrating the different components, and the index has been tested for a range of estuarine systems, differing in hydrology, tidal characteristics and pollutant load.

2. Methodology

The EQUATION index uses four different system components (Table 1), which together provide a comprehensive picture of estuarine quality. Each component is evaluated by means of a set of descriptors which are entered into the DSS. To reduce requirements (and therefore cost) of the input data, the different components are calculated using a mixed approach, relying on sampling data, the application of simple models, and heuristics.

Table 1 presents the four components and their objectives, and data requirements for descriptors. Each component is discussed below in further detail.

2.1. Vulnerability

The aim of this component is to assess the buffering capacity of a system to assimilate materials discharged into it, and to evaluate the role of internal processes compared to throughput. It provides a measure of the extent to which pollutants will be modified or recycled internally, or exported to the coastal zone. The main premise for this component is that anthropogenic input originates in the estuarine perimeter and the basins of affluent rivers, and that the coastal zone acts as a sink of pollutants existent in the estuary rather than a source.

Only one of the input variables (Tables 1 and 2) requires sampling, to provide the river flow data. This and other data are generally available, and are the input used to calculate the following descriptors, which together make up the index for this component (Table 2):

(i) Freshwater residence time (T_r) : The freshwater residence time is calculated using classical equations [21] by computing the ratio V_f/Q , where V_f is the freshwater

Component	Objectives	Data requirements for descriptors
Vulnerability	Quantify system buffering capacity	Physiography (volume, surface area, river inflow, tidal range, tidal regime, communication with ocean)
Water quality	Determine trophic balance based on nutrients, primary productivity and oxygen	Watershed information (population, watershed area) Primary production and nutrient indicators (mean chlorophyll <i>a</i> , yearly net primary production, mean nutrient concentration in river discharge) Reference parameters (mean salinity, temperature and dissolved oxygen)
Benthic quality	Evaluate status of benthos, in terms of biological communities, contamination, and bioaccumulation	Sediment contamination (estimated area affected) Bioaccumulation (excess over reference values) Benthic biomass and diversity, and equilibrium between epi/infauna (heuristic data, e.g. high/medium/low, present/absent)
Trophodynamics	Assess trophic web equilibrium based on ichthyofaunal data	Fishing and aquaculture activity, Quality of fish products, Fish diversity, Nursery areas (heuristic data, e.g. high/medium/low, present/absent)

Table 1 EQUATION index components, objectives and data requirements

volume in the estuary and Q is the inflow. $V_{\rm f}$ is calculated from the estuary volume and mean salinity, which is part of the data requirement for the *Trophic status* component. A long freshwater residence time implies the permanence and transformation of pollutants in the system.

(ii) Estuary number (E_n) . The estuary number is calculated as the ratio Q/T_p , where T_p is the tidal prism, expressed as a percentage. It is included as a descriptor of the vulnerability index as an indicator of vertical stratification. This approach is similar to the dissolved concentration potential (DCP) approach for susceptibility to nutrients [22], which uses the ratio of freshwater volume and freshwater inflow: Low values of DCP suggest that the estuary has a "significant dilution ability" [22].

Care must be taken when analysing estuary number results, since pronounced vertical stratification may have implications in the oxygenation of bottom water, and will mean that the water residence time calculated in (i) will be overestimated.

(iii) Coastal exchange (C_e). The degree of mixing of the estuary with adjacent coastal water may be determined as the ratio T_p/V , where V is the estuary volume, providing an

Table 2

Component	Data items	Descriptors and objectives
Vulnerability	Seven items Sampling required for river inflow	Freshwater residence time (measures flushing of discharges) Estuary number ^a (measures vertical stratification) Tidal prism : volume ratio (measures relevance of tide to the system) Time closed over the year (measures free exchange with ocean)
Water quality	Six items Sampling required for all	DIN concentration, both conservative and non-conservative (measures eutrophication) Percentage of oxygen saturation (direct measure of water quality)
Benthic quality	Five items Sampling required for all	Sediment contamination (measure of persistent pollutants, such as heavy metals and/or organochlorines) Bioaccumulation (measure of transfer of pollutants to the food chain) Biodiversity (measure of biological condition of the benthos)
Trophodynamics	Five items Sampling required for diversity and nursery areas	Fishing and aquaculture activity (measure of primary sector interest in the system) Quality of fish products (related measure of economic value of the system) Fish diversity (measure of the stability at the top of the trophic web)

Descriptors for each component and their objectives (shown in parantheses), and number of data items required (see text for further details)

^aSensu Hansen and Rattray [3].

indicator of the turnover of the water mass as a whole (or of the influence of the coastal zone on the estuary).

These descriptors are assigned values of 1 (worse)-5 (better), based on the criteria shown in Table 3, and an overall mixing index (M_i) is calculated as the average of $T_r + E_n + C_e$.

(iv) Proportion of time closed to the ocean (C_o). The validity of descriptors (i) to (iii) is conditioned if there are significant periods of time during which no free connection to the coastal ocean exists, as is sometimes the case in coastal lagoons. The previous descriptors are combined with the proportion of time closed to the ocean according to a heuristic matrix (Table 4), in order to provide a final grade for this component. The scoring system was designed to include "cut-off" points for grades 1 and 2 (bad and low) for both M_i and C_o : e.g. a score of 1 for either metric would automatically result in combined grade of 1 (bad).

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Grade	Residence time (days)	Estuary number (%)	Coastal exchange	
5 (better)	< 10	≤1	≤1	
4	< 20	≤ 10	≤ 10	
3	< 30	≤ 25	≤ 35	
2	< 40	≤ 100	≤ 70	
1 (worse)	≥ 40	> 100	> 70	

Grading for residence time, estuary number and coastal exchange (categories determined heuristically)

Table 4

Classification matrix for vulnerability component. The upper part of the table shows the combinations of M_i (where $M_i = (T_r + E_n + C_e)/3$), and closure to ocean C_o which correspond to different scores. The lower part shows the possible combination matrices

Grade Metric	1 (Bad)	2 (Low)	3 (Fair)	4 (Good)	5 (Excellent)
$ M_{i} \\ C_{o} (\%) $	$M_{\rm i} \ge 1$ $C_{\rm o} > 75$	$\begin{array}{l} M_{\rm i} \geqslant 2 \\ 50 < C_{\rm o} \leqslant 75 \end{array}$	$\begin{array}{l} 3 \leqslant M_{\rm i} < 5 \\ 25 < C_{\rm o} \leqslant 50 \end{array}$	$M_{\rm i} \ge 3$ $0 < C_{\rm o} \le 25$	$\begin{array}{l} M_{\rm i} \geqslant 4 \\ C_{\rm o} = 0 \end{array}$
Metric		Combination n	natrix		Grade
M _i C _o		4 5 5 5 4 5			Excellent (5)
$M_{ m i}$ $C_{ m o}$		3 4 5 5 4 3			Good (4)
Μ _i C _o		$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$			Fair (3)
$M_{ m i}$ $C_{ m o}$		$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3 4 5 2 2 2 2		Low (2)
Μ _i C _o		$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	1 2 3 4 5 5 1 1 1 1		Bad (1)

2.2. Water quality

The aim of this component is to provide an image of the estuarine water column, focussing on eutrophication and oxygen status. Although these descriptors are logically interrelated, they are evaluated separately and then combined using the matrix approach described for the *Vulnerability* component.

Table 3

2.2.1. Eutrophication

Eutrophication potential is computed using a simple steady-state model [23], modified to take into account tidally induced dispersion. Because nitrogen is frequently the limiting nutrient in estuaries, dissolved inorganic nitrogen (DIN: $NH_4^+ + NO_2^- + NO_3^-$) is used as an indicator, although phosphorus may be included as a limiting factor. The change in nitrogen mass in the estuary is described by

$$\frac{\partial M_{\rm w}}{\partial t} = M_{\rm in} - \sigma M_{\rm w} - M_{\rm out},\tag{1}$$

where $M_{\rm w}$ the mass of nitrogen in the estuary, t the time, $M_{\rm in}$ the nitrogen loading to the estuary, σ the non-conservative sink term and $M_{\rm out}$ the nitrogen discharge from the estuary.

 M_{out} is composed of an advective outflow term and a dispersive exchange term:

$$M_{\rm out} = m_{\rm out} v_{\rm out} + k_{\rm e,s} (m_{\rm w} - m_{\rm sea}), \tag{2}$$

where m_w is the nitrogen concentration in the estuary, m_{out} the nitrogen concentration in the outflow (= m_w for a one box model), v_{out} the advective outflow (= river inflow), m_{sea} the nitrogen concentration in the ocean and $K_{e,s}$ the bulk dispersion coefficient between the estuary and ocean.

Considering that for a sufficiently large integration period (e.g. over a year) $\delta M_w/\delta t = 0$, and dividing by the estuary volume, Eq. (1) may be rewritten as

$$m_{\rm w} = \frac{M_{\rm in} + k_{\rm e,s} m_{\rm sea}}{V(\sigma + \rho) + k_{\rm e,s}},\tag{3}$$

where V is the estuary volume and ρ the estuary flushing rate (inflow/volume $= v_{out}/V$).

Since $M_{in} \gg k_{e,s}m_{sea}$, Eq. (3) is further simplified (Eq. (4)), dispensing with the need for the DIN concentration in the sea (m_{sea}) ,

$$m_{\rm w} = \frac{M_{\rm in}}{V(\sigma + \rho) + k_{\rm e,s}} \,. \tag{4}$$

The non-conservative sink term for nitrogen (σ) is calculated as the phytoplankton production/biomass ratio (biomass turnover), and therefore data for the yearly net primary production and mean biomass (expressed as chlorophyll *a*) are required. Other data are obtained from input data to the vulnerability component, and the nitrogen load is estimated based on the *per capita* discharge. The value obtained for m_w assumes that all the primary production is a dissolved nitrogen sink, but this is unrealistic, because although some particulate nitrogen is exported to the coastal zone by estuarine flushing, a part is returned to the estuary as DIN due to mortality of phytoplankton and higher trophic levels and subsequent mineralization processes. The results from this component therefore also consider the theoretical nitrogen concentration in a conservative situation and the conservative and non-conservative DIN concentration values are averaged to provide a final value for m_w . The nitrogen loading to the estuary from river discharges may optionally be included (added to) the load associated with the population (or equivalent) around the estuary perimeter. The possibility of switching on/off this component in the DSS provides an indicator of the relative importance of local discharges and the river basin contribution.

2.2.2. Oxygen saturation

Oxygen saturation is determined from the mean dissolved oxygen concentration, normalised using the average salinity and temperature data, and a set of five categories is defined (Table 5). The dissolved nutrient concentration estimated from the model is associated to the oxygen saturation descriptor to provide an overall grade for this component. The matrices are shown in Table 5, and, as for the vulnerability component, the combinations have been optimised in order to provide a weighting system for high DIN or low oxygen saturation values to lower the index independently (e.g. 1:5 and 5:1). Some of the partial index combinations are unrealistic (e.g. it is unlikely that low dissolved nutrients co-exist with very low oxygen) but the DSS does not explicitly implement checks for this.

2.3. Sediment quality

The aim of this component is to examine the sediment and benthos using three different descriptors to provide an overall measure of quality. The descriptors are

Table 5 Grading for trophic status component (5 — better; 1 - worse). The upper part of the table shows the combinations of nitrogen concentration (m_w) and % saturation of dissolved oxygen (% O₂) which correspond to different scores. The lower part shows the possible combination matrices 1 (Bad) 2 (Low) Grade 3 (Fair) 4 (Good) 5 (Excellent) Metric m_w^a $m_{\rm w} > 70$ $70 \ge m_w > 40$ $40 \ge m_w > 25$ $25 \ge m_w > 10$ $m_{\rm w} \leq 10$ $O_2 < 35$ $35 \leq O_2 < 50$ $50 \le O_2 < 65$ $65 \leq O_2 < 80$ $O_2 \geqslant 80$ O₂ (%) Metric Combination matrix Grade 4 5 5 Excellent (5) m_w 5 4 5 $%O_2$ 3 5 4 Good (4) m_w 5 4 $%O_2$ m_{w} 3 3 Fair (3) 3 3 $%O_2$ 2 1 2 1 2 4 5 Low (2) m_{w} 4 5 3 4 5 2 2 $%O_{2}$ 1 2 2 3 3 5 Bad (1) 1 1 4 m_w 1 2 3 2 1 2 1 1 $%O_2$ 1

^a m_w : mean nitrogen concentration in µmol1⁻¹, category ranges adapted from NOAA [43].

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evaluated by the user on the basis of expert knowledge of the ecosystem, which implies that there are quantitative or semi-quantitative data available. The index for this component is calculated by aggregating three metrics: The area of contaminated sediments in the system, the bioconcentration of xenobiotics in bivalve filter-feeders, and a combined measure of the equilibrium of the benthic communities.

For this index (unlike the previous two components) scores are given according to observed distributions, and no direct calculations are performed. For this reason, the results are presented graphically, either as a histogram or as a tri-axial plot displaying aggregated ratio-to-reference values. The latter approach has been previously used e.g. by Chapman [10] as a representation of the sediment quality triad. Wherever samples are combined to provide an indicator value at one station, a percentile-based approach is used, rather than mean values, to reduce the weight of potential outliers [13]. Details for the three metrics used to assess sediment quality are provided below.

2.3.1. Persistent pollutants

Sediment concentrations (particularly in fine-grained material) provide a good signal for the discharge of persistent pollutants such as heavy metals or organochlorine compounds [24,25], but high concentration areas are conditioned by transport processes, and are usually relatively confined [26]. A useful descriptor of sediment quality is thus the area affected by pollution, which will indicate the degree of spatial contamination of an estuary. In order to determine the affected area, a probabilistic approach has been adopted, based on a division of the system into a set of grid cells, and on contamination levels defined using sediment quality guidelines for the protection of aquatic life [13,27]. The criteria for contamination follow Long et al. [14] and previous authors, and are based on probable effect levels (PEL), representing concentrations above which effects are more frequently observed. Arsenic, cadmium, lead and mercury were chosen as indicators of metal pollution, and DDT and PCBs as representative organic micropollutants. Table 6 shows PEL values for these substances, as well as Action Level/Level of Concern values which are used for other metrics. For each grid cell, the median value for each sampling station is determined, and if any of the PEL values for indicator contaminants are exceeded, the station is considered polluted. The contamination of a grid cell is based on the proportion of contaminated stations contained: e.g. if 4 stations exist, and one of these exceeds PEL values, the grid cell is considered 0.25 contaminated and 0.75 uncontaminated. This approach addresses two of the key questions regarding sediment contamination, i.e. "What is the nature and spatial extent of chemical contaminants in sediments relative to appropriate reference conditions?" and "What sediments have sufficiently high concentrations of chemical contaminants so as to present unacceptable risks to humans or aquatic biota?" [28].

The procedure for grading areal contamination of sediments is illustrated in Fig. 1 and Table 7. The main concern was to develop a methodology which may be applied in a simple form, but maintains comparability between different systems. The classification of areal contamination may be carried out using a geographical information system (GIS), on which the sediment stations and respective median values are marked. Alternatively, if this is not available, a square grid containing at least 10 cells Table 6

Parameter	PEL ^a Metals in mg kg ⁻¹ , organochlorines in μg kg ⁻¹	Background concentration in molluscs ^b (mg kg ⁻¹)	Background concentration in fish ^e (mg kg ⁻¹)	Action Level or level of Concern ^d (mg kg ⁻¹)
Arsenic	41.6	1.5 (oysters)	3.34	86°
Cadmium	4.2	0.067 (clams)	0.01	4 ^e
Lead	112	0.09 (ovsters)	0.01	1.7 ^e
Mercury	0.70	0.02 (cockles, mussels & scallops)	0.06	1^{f}
DDT	4.77	0.002 (unspecified)	0.01	$5^{\rm f}$
PCBs	189	0.02 (unspecified)	0.02	2 ^g

Probable effect levels (PEL) for metals and organic pollutants in marine sediments, reference concentrations in shellfish and fish, and Action Levels or Levels of Concern for shellfish and fish

^aEnvironment Canada [27] and MacDonald et al. [13].

^bUSFDA [30-33]; MAFF [34,35].

^eMetals: median for 110 samples of cod, haddock, herring, mackerel, plaice, redfish and whiting [35]. Organochlorine compounds: median for 16 samples of deep water fish [36].

^dUSFDA[30-36].

^eLevel of Concern.

^fAction Level.

^gTolerance.

is superimposed on an estuary map (Fig. 1) and the system is graded based on the distribution of contaminated and uncontaminated cells. Several requirements must be met in order to allow a valid comparison between systems. First, interpolation of station values should not be carried out, since the premise of this approach is that the sediment pollution is restricted to confined areas [26]. Second, the concentration values used should not be normalised (e.g. according to grain size) because the object is to determine effect levels on the biota. Thirdly, at least 75% of the grid cells which contain water must have one station or more, and at least 75% of the total cells considered must contain water, in order to ensure adequate system coverage.

With reference to Fig. 1 and Table 7, two idealized cases are represented, estuaries A and B. In each case, scenarios are presented for 30 grid cells, 10 grid cells and 1 grid cell (i.e. the whole system — shown only in Table 7). The contaminated area given by this method is fairly independent of the number of grid cells used, even in situations where less than 75% of the cells contain sampling stations. For cases where one station exists per grid cell or where all the stations are confined to one grid cell the contaminated area given will be identical, but the probability (*p*) of occurrence is very low ($p = N!/[(N - S)!N^S]$ with N the number of grid cells, S the number of stations, and $p = 1/N^{(S-1)}$, respectively).

In the B1 example, not enough cells exist to provide a reliable estimate of contamination, and in B2, the estimate is improved due to more homogeneous station distribution. The case (Table 7) where the whole system is one cell only is obviously



Fig. 1. Schematic grid division of different estuaries for determination of contaminated sediment area. Table 7

Case		A1			A2			B1			B2	
Grid size (cells) Samples suggest:	30	10 Pollut	1 ed	30 L	10 Jnpolli	1 uted	30	10 Pollut	1 ed	30 U	10 npollu	1 ited
No. contaminated cells	6	5.5	0.89	1	1	0.11	4	2.75	0.71	4	1.9	0.29
No. uncontaminated cells	1	0.5	0.11	6	5	0.89	2	1.25	0.29	12	6.1	0.71
No. water cells	25	8	1	25	8	1	26	9	1	24	9	1
No. unsampled cells	18	2	0	18	2	0	20	5	0	8	1	0
% polluted cells % system covered	86% 28%	92% 75%	89% 100%	14% 28%	17% 75%	11% 100%	67% 23%	69% 44%	71% 100%	25% 67%	24% 89%	29% 100%

Sample results of a probabilistic approach to determine the proportion of contaminated cells

not applicable, and is only shown to illustrate that the result for contamination shows little dependence on grid size even in an extreme case.

In the present index five grades are defined (Table 8), ranging from light contamination to gross pollution. The values for areal contamination are calculated as the ratio

Grade	Persistent pollutants	Bioaccumulation ratio C _i
5 (better)	Localised ($< 10\%$ of area)	$C_i \leq 1$
4	Moderate (10-30% of area)	$1 < C_i \leq 5$
3	Heavy (30–50% of area)	$5 < C_i \leq 10$
2	Widespread (50-70% of area)	$10 < C_i \leq \text{Action Level}^a/\text{Reference}$ concentration
1 (worse)	Gross ($> 70\%$ of area)	$C_i \ge Action Level^a/Reference concentration$

Grading for persistent	pollutants in the sediment	t and bioaccumulation

^aOr Level of Concern.

of contaminated cells to total sampled cells (i.e. contaminated + uncontaminated cells).

Although the cost of this type of analytical data is high, and one of the objectives of the EQUATION index is to optimize the cost-benefit of the information used, generic quantitative knowledge of this type already exists for many estuaries. Furthermore, the rate of change of persistent pollutants in the sediment is usually low, which means that a dataset gathered over a period of time (e.g. a decade) in different parts of the system will probably be adequate, eliminating the need for dedicated synoptic sampling.

2.3.2. Bioaccumulation

The sediment area affected by persistent pollutants is a measure of the spatial scope of pollution, but not of its magnitude. The concentration of metals or organochlorine compounds in the sediment varies not only with discharge but with hydrodynamics, grain size and organic content. The bioavailaibility of xenobiotics is difficult to assess from sediment contamination [13,29], because it is conditioned by transformations occurring in the sediment, sediment–water interface and water column, which may be biologically mediated. Laboratory toxicity tests may be used [14], or field data regarding community composition or bioaccumulation. However, there is some difficulty in relating persistent pollutants to community composition, particularly in estuaries where factors such as temporal salinity gradients strongly influence the make-up of the benthos. In this index, the magnitude of persistent pollution is determined from the bioaccumulation in key benthic species.

The substances selected are identical to those used for the sediment analysis, i.e. As, Cd, Pb, Hg, DDT and PCBs. The criteria for defining the classes given in Table 8 were defined on the basis of the reference values for contaminants in shellfish and on the Action Levels/Levels of Concern for these substances provided in the literature [30–36]. Where reference concentrations were available for more than one type of shellfish, the lower value was selected. Five classes were defined (Table 8): At or below the reference value (score 5 — better), up to 5 times the reference value (score 4), up to

Table 8

		,			
Contaminant	$C_{\rm i} \leqslant 1$	$1 < C_i \leq 5$	$5 < C_{\rm i} \leq 10$	$10 < C_{\rm i} \leqslant {\rm AL^a/SRC}$	$C_{\rm i} > {\rm AL^a/SRC}$
Arsenic	1.5	7.5	15	86	86
Cadmium	0.067	0.335	0.67	4	4
Lead	0.09	0.45	0.9	1.7	1.7
Mercury	0.02	0.1	0.2	1	1
DDT	0.002	0.01	0.02	5	5
PCBs	0.02	0.1	0.2	2	2
Score	5	4	3	2	1

Concentration upper limits in mg kg⁻¹ fresh weight, corresponding to C_i scores (AL — Action Level, SRC — Shellfish Reference Concentration)

^aOr Level of Concern.

Table 9

10 times the reference value (score 3), up to the Action Level or Level of Concern value (score 2), and above the Action Level/Level of Concern (score 1).

The scoring category is calculated as C_i , defined as the ratio B_p/R_p , where B_p is the concentration in the indicator bivalve and R_p is the baseline concentration for the same species. The concentration ranges corresponding to the C_i classes are shown in Table 9. Median values for shellfish should be used, based on samples from fishery areas or regular monitoring programmes. Where results for several contaminants are available, the precautionary principle should be applied by using the highest concentrations relative to Action Levels of Concern.

2.3.3. Biodiversity

The last descriptor in this component is the benthic biodiversity, which is approached using the same type of heuristically defined grade matrix as described previously. The biodiversity descriptor is made up of three parts, community diversity, community biomass, and the presence/importance of infauna and epifauna (Table 10). The premise on which this descriptor rests is that increased diversity is desirable, as is the presence of epifauna and infauna (balanced groups). A high benthic biomass will weigh negatively on the index if the diversity is low, and some combinations of diversity/biomass/balance are considered inapplicable. In such cases the DSS will use default values for this descriptor.

2.4. Trophodynamics

The last component of the index is based on the concept that higher trophic levels provide an integrated measure of the quality of an ecosystem, although by themselves they will not provide a sufficiently complete diagnosis. The previous three components do not relate directly to the community at large, although some events have a direct impact on the users of the system, e.g. hypoxic or anoxic conditions leading to fish kills or odour problems, or interdiction of bivalve consumption due to toxic algal blooms.

Metric	Combination matrix	Grade
Biomass Diversity	2 2 1 1 0 0 2 2 2 2 2 2 4 4 5 4 5 4	Excellent (5)
Balance Biomass Diversity Balance	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Good (4)
Biomass Diversity Balance	$\begin{vmatrix} 2 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{vmatrix}$	Fair (3)
Biomass Diversity Balance	2 1 0 0 2 2	Low (2)
Biomass Diversity Balance	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Bad (1)
Biomass Diversity Balance	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Inapplicable

Grading for biodiversity component (2 — better; 0 — worse). Matrix top row: biomass; middle row: diversity; bottom row: balance

The basis for this component is that the uses of a system reflect its quality, and therefore that simple metrics related to the importance of different uses provide a suitable assessment of the ecosystem value. The focus is on fish and fishing, both from fisheries and from a recreational standpoint.

Four descriptors were chosen: fishing and aquaculture activity, quality of fish products, fish diversity, and nursery aspects. For the first two descriptors, fish are considered to include finfish, shellfish, and other commercially important fishery products. The categories for classification are shown in Fig. 2 and the descriptors are examined in more detail below.

2.4.1. Fishing and aquaculture

The quality of an estuarine system is reflected in the types and range of human activities associated with it. Fishing and aquaculture indicate the importance of the renewable resources, both in terms of abundance and diversity, and are thus used as

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Table 10



Fig. 2. Trophodynamics component of the DSS, showing sliders for setting grades and category descriptions.

a descriptor, using five qualitative categories of importance, ranging from 5 (abundant fishing and/or aquaculture) to 1 (fishing and aquaculture practically inexistent).

2.4.2. Fish quality

The quality of the resource, described qualitatively in terms of taste and quantitatively in terms of levels of persistent pollutants, can be combined with the previous descriptor to indicate the value of primary sector activity in an estuary. The quantitative basis for this metric is the contamination by persistent pollutants. With reference to Table 8, a similar methodology to that employed for shellfish classification is used, based on reference concentrations and Action Levels/Levels of Concern for 4 metals and 2 organochlorine compounds. Table 11 shows the limit values for the C_i metric and corresponding scores. For organoleptic quality, the categorization must be heuristic, and will affect the overall trophodynamic metric by allowing a one-point shift in classification (i.e. it has a weight of 20% of the contaminant metric).

2.4.3. Fish diversity

The species diversity is an accepted indicator of the robustness of the trophic web, not only in terms of degradation of environmental conditions due to emissions, but also as a sign of instability due to excessive monoculture. Therefore, a system where

Contaminant	$C_{\rm i} \leqslant 1$	$1 < C_i \leq 5$	$5 < C_{\rm i} \leqslant 10$	$10 < C_i \leq AL^a/FRC$	$C_{\rm i} > {\rm AL^a/FRC}$
Arsenic	3.34	16.7	33.4	86	86
Cadmium	0.01	0.05	0.1	4	4
Lead	0.01	0.05	0.1	1.7	1.7
Mercury	0.06	0.3	0.6	1	1
DDT	0.01	0.05	0.1	5	5
PCBs	0.02	0.1	0.2	2	2
Score	5	4	3	2	1

Concentration upper limits in mg kg⁻¹ fresh weight, corresponding to C_i scores (AL — Action Level, FRC — Fish Reference Concentration)

^aOr Level of Concern.

only a few species are relevant (perhaps because of a highly focussed intensive aquaculture) will score badly in this category. Clearly, if intensive aquaculture results in organic enrichment of the sediments, other index components such as the *water quality* will also be negatively affected.

The index for this component is calculated by summation of the scores of the three descriptors, with an additional score of two if the system is classed as an important nursery area and one if the consumer acceptance of fish from the system is high. As was done for the previous component, the first three descriptors are represented in the DSS as a set of histograms (Fig. 3), where the horizontal bar indicates the overall score for this component. Alternatively, these results may be viewed as a tri-axial plot, where deviations from the reference situation are represented as enlargement and/or assymetry of a standardized equilateral triangle.

2.5. Overall representation

The final index for an estuary is calculated as the weighted sum of the four partial component indices. The mixing component is given slightly less weight than the other three components (22% for *Vulnerability* compared to 26% for the others), to avoid over penalizing an unspoilt system due to its physical constraints. The index is represented as a number ranging from 5 (better) to 1 (worse), to which is associated a colour varying from blue (better) to red (worse), following the European Union Water Quality Directive [37].

3. Results and discussion

Some results are provided of the application of the EQUATION index, based on estuaries with different characteristics, with regard to physiography, nutrient loading and industrial impact. Following a review of existing information [38–49], five cases have been chosen, two from the USA and three from the European Union, and graded based on published data.

Table 11

The input data and the results for the index are shown in Table 12. The systems which are reviewed have widely differing physical characteristics: A small coastal lough (Carlingford Lough), a small microtidal estuary (Tomales Bay), a large microtidal system (San Francisco Bay) and two large mesotidal systems (Elbe and Tagus estuaries) were considered. These systems also differ widely in nutrient loading, persistent pollutants, benthic quality and exploitable renewable resources. General features for these systems are given by many authors; indicative references for each are: Carlingford Lough [48], Elbe estuary [50], S. Francisco Bay [51], Tagus estuary [25] and Tomales Bay [47].

The visualisation of the index is shown in Fig. 3. The *vulnerability* and *water quality* components show the results of the simple models applied, and the *sediment quality*

Table 12

Input data and results for the EQUATION index for different European and North American estuaries (see methodology section for description of grading system).

Parameter	Carlingford Lough (Ireland)	Elbe estuary (Germany)	S. Francisco Bay (USA)	Tagus Estuary (Portugal)	Tomales Bay (USA)
Volume (10^6 m^3)	195	2520	6681	1900	84
Surface area (km ²)	39	351	4147	320	28
Modal river flow $(m^3 s^{-1})$	4	507	1044	400	2.85
Mean tidal range (m)	3.5	3	0.78	2.5	1
Population ($\times 10^3$)	70	5250 ^a	9000 ^a	3000 ^a	11 ^b
Mean chlorophyll $a (\mu g l^{-1})$	2.65	10	5.1	7.9	6.61
NPP (gC $m^{-2} yr^{-1}$)	12.5	127.25	23	80	480
DIN in river $(\mu mol l^{-1})$	61.5	590.3	32.3	42.3	19.1
Mean salinity	29.89	4	20.33	22.75	32.70
Mean water temperature (°C)	9.85	11.5	15.76	17.30	14.08
Mean diss. oxygen $(mg l^{-1})$	10.4	6.5	8.24	7.3	7.5
Areal sediment contamination	5	1	5	4	5
Bivalve bioaccumulation	5	2	2	2	5
Benthic biomass	2	1	1	1	2
Benthic diversity	2	0	1	0	2
Benthic balance	2	1	1	1	1
Fishing/aquaculture	4	2	3	3	5
Fish quality	5	2	4	2	5
Fish diversity	4	3	4	3	3
Important nursery role	0	0	0	1	1
Consumer acceptance	1	0	1	0	1
EQUATION index	Good	Low	Good	Fair	Excellent
Overall score	4	2	4	3	5

^aPopulation is multiplied by 1.5 to account for industrial discharges in the estuary watershed.

^bPopulation is multiplied by 2 to account for the cattle population in the estuary watershed.



Fig. 3. Results screen of the EQUATION decision support system (example shown for Tomales Bay).

and *trophodynamics* sections show the graphical representations. The final score is shown on the bottom right.

The results obtained for the systems tested range from low to excellent, spanning four of the five classifications. The data necessary for loading the index were found to be accessible, and enable a broad comparison of different systems to be carried out, irrespective of morphological differences. Nevertheless, some data items deserve further comments: The physical aspects required by the index are generally well covered, although care should be taken in the use of a modal river discharge rather than a mean value, to avoid bias in the case of "torrential" discharge behaviour, which occurs in the Tagus estuary and S. Francisco Bay, but not in the north European systems, where rainfall is more regular. Estimates of population are difficult because the concept behind the nitrogen loading model is based on per capita loading for population equivalent (PEQ) which includes industrial and/or agricultural inputs. For this reason, the Tagus, S. Francisco Bay and Elbe populations were revised upwards by 50%, (which in the case of the Elbe is probably too low) and Tomales Bay was doubled to account for cattle, which outnumber the human population.

The validation of the index was done in three ways: First, the index results were compared heuristically with expert evaluation, and good agreement was obtained. Second, the results of the nutrient model were compared with mean values calculated from measurements in each system (Fig. 4). The measured values correlate well with



Fig. 4. Comparison of measured and calculated values for DIN in four of the test systems.

the nutrient model (r = 0.97, p < 0.05) though the model underestimates the measured data by about 30%. Changes to the PEQ estimates described previously should improve the model results. Results for the Elbe are not shown, since a mean value for DIN in the estuary could not be established. Values at Hamburg, where salinity is below 5, can exceed 300 µmol 1^{-1} , and N : P atomic ratios can be of the order of 100, so this is clearly a highly modified system.

Thirdly, where possible, other indices were applied to the five estuaries and compared to the results obtained in this work. For the benthos, comparisons could not be carried out due to the data requirements of other indices [15,18,19], but there is good qualitative agreement with available data for sediments and benthic organisms for the Elbe [52], San Francisco Bay [39], the Tagus [53] and Tomales Bay [54].

For water quality, a comparison was made by applying the TRIX eutrophication index [17]. Using TRIX, all the estuaries were classified in the best state (<4) except the Elbe, which rates as mediocre (5–6). In the present work, all systems except the Elbe rated a 5; the Elbe was graded 1, i.e. of poor water quality.

Parallel tests were carried out with two "conceptual" estuaries, combining low energy situations with poor-quality and high-quality scenarios, in order to test the responsiveness of the index to change. For two of the selected systems, different development scenarios were considered, to analyse the response of the index both to improvement and degradation of environmental conditions. For these scenarios, it is not possible to validate the results, but the differentiation of the test cases can be seen in Fig. 5. These results show the partial scores for the four components of the index and the resulting grade. Note that, in the figure, the final grade may differ for systems



Fig. 5. Grading of different estuaries (lower scores are worse, systems marked in italics are scenarios or conceptual systems).

with apparently identical aggregate partials. This is because only the rounded-off components are shown, but the final index is calculated from the original data. The five test systems have a score of 4 in the *vulnerability* component, for different reasons: for instance Tomales Bay has a third of the tidal range of Carlingford Lough and a lower freshwater inflow, but it has a half the volume and higher mean salinity, and both have a high exchange with the coastal zone. A closure scenario of the bay for 30% of the time will result in a score of 2 for *vulnerability*, which by itself would bring down the overall grade to 4 (good). However, it is not possible to consider scenarios in this form, because other input variables such as dissolved oxygen would also change, further lowering the overall grade. Although the *vulnerability* score in the five systems is identical, the physical differences between the various systems are reflected in the water quality grade because the population data, volume and river flow are all inputs to the nutrient model.

Some limitations to the index may be identified, as well as possible improvements. An effort was made in the development of the concept and implementation of the software to limit highly improbable or impossible combinations of input data, but there is always potential for misuse, either through bias or errors in the data. For benthic quality and higher trophic levels, some of metrics use quantitative assessments of scope and magnitude of contamination, through Probable Effect Level and Action Level or Level of Concern values; others depend on an expert-based heuristic approach, as occurs in other evaluations [43–45], and allow comparisons in only a semi-quantitative form. Despite some reduction in comparability, there are advantages in this integrated view of estuarine quality and condition, which allows not only the inclusion of epibenthos as well as infauna, but also the consideration of socio-economic aspects.

Extreme values of water quality data (e.g. dissolved oxygen, DIN or chlorophyll *a*) are probably more relevant than mean values, because they indicate anoxic or hypoxic events, or acute eutrophication phenomena. However, for a large system like S. Francisco Bay or the Elbe estuary these responses will be localised in space, and an

overall picture of the estuary quality will be biased by the use of these criteria. Estuaries which are phosphorus limited may easily be added to the DSS, since the nutrient model is directly applicable — the additional requirement (which is not negligible) would be for the user to specify which nutrient limits production in the estuary. One possible improvement to this index is the inclusion of benthic primary producers, which could be used both as a nutrient sink in the model and as an extra measure of human impact (e.g. through estimates of saltmarsh reclamation), although practical problems might arise due to the lack of reliable data on benthic primary productivity and areal coverage.

A warning must be issued that the methodology presented in this paper is clearly not designed for detailed management of a particular system, which needs a completely different approach, focussing on specific problems and potential solutions.

The EQUATION index does synthesise the four major descriptors of estuarine quality. The physical characteristics of restricted environments such as estuaries, fjords, lochs and coastal lagoons are usually analysed through simple models; water and sediment quality are evaluated through indices, in the former case normally based on concentration ranges of stressors and in the latter on a combination of stressor concentrations and community diversity or other biotic indices. Socio-economic indicators are rarely applied in this context. The value of the present approach lies in bringing together different methodologies to provide an integrated comparative overview of different systems, taking into account a broad range of physical characteristics and water uses.

The decision support system developed for this work was implemented in C + +, runs under Windows NT/98, and is available for download, together with the test systems used, from http://tejo.dcea.fct.unl.pt/ecomod/modload.htm.

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