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Ecological Modelling xxx (2003) xxx–xxx

ECOLOGICAL MODELLING

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Performance of a stochastic-dynamic modelling methodology for running waters ecological assessment

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Received 28 January 2003; received in revised form 2 September 2003; accepted 27 October 2003

Abstract

An holistic stochastic-dynamic modelling methodology has been developed in order to predict the ecological status of lotic systems in Northeast Portugal. These procedures focus on the interactions between conceptually isolated key-components, such as some relevant benthic macroinvertebrate metrics and changes in local habitat conditions. The proposed model was preceded by a conventional multivariate statistical treatment performed to discriminate the significant relationships between prevailing biological and environmental variables. Since this statistical analysis is static, the dataset recorded from the field included true gradients of habitat changes. In this way, the factors time and space are implicit in the respective treatment. Such a procedure gives credibility to the parameters included in the dynamic model construction. In order to enhance the importance of monitoring in aquatic systems based on ecological integrity indicators, different biotic metrics were selected from the studied benthic macroinvertebrate communities. The samples of aquatic macroinvertebrate, environmental and physical-chemical data were collected from three watersheds of mountain rivers in Northeast Portugal, between 1983 and 1985. The model validation was based on independent data from another watershed not included in the model construction. Thereafter, the model behaviour was tested facing a "new" scenario, namely ongoing organic pollution disturbances in the region. The results are encouraging since, after the model validation, they seem to demonstrate the reliability of the model (1) to assess the ecological status of running waters from the studied watersheds and (2) to predict the behaviour of key macroinvertebrate metrics, along an ecological gradient from relatively pristine conditions to serious human impacts.

Keywords: Running waters; Aquatic ecosystem integrity; Ecological indicators; Aquatic macroinvertebrates; Stochastic-dynamic modelling; Holistic approaches

1. Introduction

The ability of humans to change the world outpaces the capacity of living systems to respond to those changes (Dolèdec et al., 1999; Kimberling et al., 2001). Therefore, most of the freshwater lotic ecosystems are subject to severe pressure by either an alteration in the quality or the quantity of the water, as well as the structure of these systems. This pressure forces changes in biotic communities, especially evidenced in a reduction of their characteristic biological diversity (Ribaudo et al., 2001; Harris, 2002). The progressive degradation of running waters takes place in most watersheds in Northeast Portugal (Cortes, 1992).

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0304-3800/$ – see front matter © 2003 Published by Elsevier B.V.
doi:10.1016/j.ecolmodel.2003.10.021

For conservation and management purposes, the use of adequate ecological integrity indicators is particularly helpful in assessing the impact of environmental changes on characteristic ecological patterns (Barbour et al., 1999; Dolèdec et al., 1999; Rabeni, 2000; Andreasen et al., 2001; Dale and Beyeler, 2001; Karr and Rossano, 2001; Kurtz et al., 2001; Karr, 2002). Ecological integrity is a concept centered in the system as a whole, but depends on the state of all components, such as the presence of species, populations and autochthonous communities, the occurrence of appropriate ecological processes and the maintenance of all the environmental conditions that support the ecosystem (Angermeier and Karr, 1994; Townsend and Riley, 1999; Dale and Beyeler, 2001). Since ecological indicators can reflect biological, chemical and physical aspects of ecological conditions, they have been used to characterize status, to track or predict changes, to identify stressors or stressed systems, to assess risk and to influence management actions (Seager, 1999; Rabeni, 2000; Karr and Chu, 2001; Kurtz et al., 2001; Karr, 2002). The biological alterations due to extrinsic causes or inherent in the natural running of aquatic ecosystems can be considered at the molecular or physiologic level, at the individual level and at population or community levels (Cortes, 1992; Karr, 1998, 1999; Turak et al., 1999; Cortes et al., 2002). Key aquatic communities have been used, in some cases for decades, to evaluate the biological quality of streams, rivers and lakes (Karr, 2002).

In this paper, the macroinvertebrate communities were used as ecological integrity indicators of aquatic ecosystems. These communities have been commonly chosen for aquatic bioassessment investigations as aquatic invertebrates respond rapidly to environmental changes and provide signs for the early detection of ecological changes (Barbour et al., 1999; Kimberling et al., 2001). They are present in wide aquatic habitat types, possess life cycles with a relatively long aquatic phase giving information on short and long term disturbances and are relatively easy to sample and process due to their conspicuous nature (Wright et al., 1989, 1992; Hutchens et al., 1998; DeWalt et al., 1999; Whiles et al., 2000). Additionally, great progress has been made towards standardized methods of collection and analysis of these groups (Barbour et al., 1999; Karr and Rossano, 2001; Cortes et al., 2002). Other advantages of macroinvertebrate communities are related to the capacity for population recovery in response to good management procedures in previously disturbed ecosystems (Cortes, 1992; Barbour et al., 1999; Harris and Silveira, 1999; Karr, 2002). This recovery depends on countless factors such as the duration and nature of the disturbance, characteristics of the organisms (namely the life cycle phase) and the capacity of recolonization of affected habitats (Wallace, 1990; Yount and Niemi, 1990; Mackay, 1992; Hutchens et al., 1998; Rabeni, 2000; Kurtz et al., 2001). Therefore, several studies have demonstrated the effectiveness of invertebrate bioassessment for detection of stream reaches impaired by a variety of point and non-point source pollutants (see Lenat, 1998; Thorne and Williams, 1997; Karr, 1999, 2002; Maxted et al., 2000; Whiles et al., 2000; Kurtz et al., 2001).

One of the great challenges in ecological integrity studies is to predict how anthropogenic environmental changes will affect the abundance of species, guilds or communities in disturbed ecosystems (Andreasen et al., 2001). Although ecological models have been used to predict macroinvertebrate species responses to environmental stresses and habitat characteristics, most of them are static (e.g. Wright, 1995; Parsons and Norris, 1996; Kay et al., 1999; Marchant et al., 1999; Moss et al., 1999; Smith et al., 1999; Turak et al., 1999; Charvet et al., 2000; Oberdorf et al., 2001). Static models with fixed parameters are unable to estimate the structural changes when the habitat conditions are substantially changed (Jørgensen and Bernardi, 1997). Therefore, it is a goal of ecological modelling to construct dynamic models and structural dynamic models that can adequately capture the structure and the composition, including the related processes, of those systems (Jørgensen, 1994, 2001; Chaloupka, 2002). In fact, dynamic models are very important tools with which to improve the assessment of the medium- and long-term directional environmental disturbances in perturbed ecosystems (Jørgensen and Bernardi, 1997; Ault et al., 1999; Brosse et al., 2001; Cabral et al., 2001; Costanza and Voinov, 2001; Jørgensen, 2001; Voinov et al., 2001; Santos and Cabral, submitted). The application of dynamic ecological models can synthesize the pieces of ecological knowledge, emphasizing the need for an holistic view of a certain environmental problem (Mitsch and Jørgensen, 1989).

The aim of the present paper is to develop an holistic, simple, expedite and applicable methodology, by using appropriate statistical and dynamic modelling techniques, in order to contribute to the assessment of the ecological status in running waters systems. A stochastic dynamic model was constructed and validated by focusing on the interactions between conceptually isolated key-components in such systems, namely between biological metrics and physicochemical conditions. These specific components of ecosystem integrity are intricately linked by their dependence on habitat characteristics, particularly their occurrence related to environmental conditions. Hypotheses to be tested include: (1) that the selected metrics are representative of the local macroinvertebrate community that changes in some predictable way with the increase of human influence; and (2) that the ecosystem integrity can be assessed by the state variables, assumed as important ecological indicators, used in the dynamic model construction. These hypotheses were tested by new applications of a stochastic dynamic model in order to capture, in an holistic perspective, the complexity of some ecological processes resulting from the gradients of the ongoing environmental changes in the studied watersheds of Northeast Portugal.

2. Methods

2.1. Study area

The study was carried out in four main streams from the Douro river watershed, located in Northeast Portugal: the Olo (O), Corgo (C), Pinhão (P) and Tinhela (T) rivers (Fig. 1). The watersheds of these rivers have different lithological, topographical, hydrological and land use features. The studied streams range from 2nd to 10th in order of altitude (50–1500 m). The granite and schist bedrocks create a common pattern of acid and soft waters. Strongly seasonal irregular discharges, related to the precipitation pattern and low retention time are important characteristics. Land use reflects the topographical conditions: the steep slopes are covered with rough pastures mixed with forests of pine

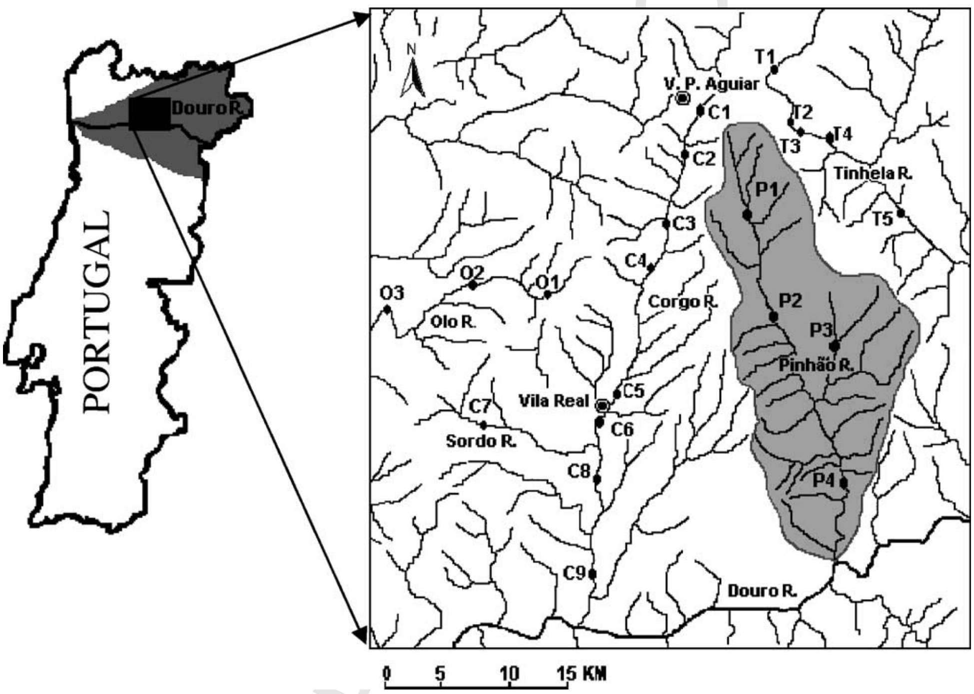

Fig. 1. Location of the study area in Northeast Portugal (shaded area) with the different watersheds used in the construction of the model (Olo (O), Corgo (C) and Tinhela (T) rivers) and in the respective validation (Pinhão river (P)).

trees; few arable crops, using a small amount of fertilizers and large areas of vineyards are present in the lower lands. During the sampling period (1983–1985) some sources of disturbance have changed these features: an input of As, Zn and sulphates, resulting from spoil heaps created by gold mines have affected the Tinhela river, and sewage from urban areas has caused eutrophic conditions in the Corgo river.

2.2. Field programme

The environmental and biological data used to support the model construction was collected in 15 sampling stations from three watersheds (O, C and T, Fig. 1) (Cortes, 1992), representative of the typological variations in the studied region. The model was validated with independent data from four sampling stations (P1, P2, P3 and P4) located in the Pinhão watershed (Fig. 1). Sampling was carried out from March 1983 to November 1985. Four sampling campaigns were made annually, corresponding to spring, summer, autumn and winter periods (see Cortes, 1992 for details). In each campaign, semi-quantitative biological samples were taken monthly in each sampling station. Therefore, the recorded data allowed to incorporate into the model the seasonality of the natural variations that occurred in these aquatic systems. Aquatic macroinvertebrates were identified at species level with the exception of Acari (presence/absence), Oligochaeta (Family) and Chironomidae (sub-Family), and grouped in relevant metrics. The data were analysed according to measures of taxa richness, composition and tolerance to environmental disturbance. These biomonitoring metrics were used to assess river health as they reveal high sensitivity to environmental stress (see, Cortes, 1992; Thorne and Williams, 1997; Barbour et al., 1999; Harris and Silveira, 1999; Karr, 1999, 2002; Maxted et al., 2000). The specifications of all physicochemical and biological variables considered in this study are presented in Table 1.

2.3. Data analysis

The stochastic dynamic model proposed is preceded by a conventional multivariate statistical procedure. A stepwise multiple regression analysis (Zar, 1996) was used to test relationships between the biological metrics and the environmental variables. The dependent variables correspond to the selected metrics expressed in number of species, with the exception of Chironomidae in sub-families. The independent variables were the environmental parameters displayed in Table 1. A step down procedure was used so that the effect of each variable in the presence of all others could be examined first, with the least significant variable being removed at every step. The analysis stopped when all the remaining variables had a significance level $P < 0.05$ (Zar, 1996). Although the lack of normal distribution of the dependent variables was not solved by any transformation (Kolmogorov–Smirnov test), the linearity and the homoscedasticity of the

Table 1
Specification (units and taxa resolution) of all physicochemical and biological variables considered in this study

Variables	Specification	Code
Environmental variables		
Alkalinity	meq. l^{-1}	ALK
Altitude of the site	m	ALT
Biochemical oxygen demand	mg O_2 l^{-1}	BOD_5
Chemical oxygen demand	mg O_2 l^{-1}	COD
Chlorides	meq. l^{-1}	CL
Conductivity at 20 °C	µmhos cm^{-1}	COND
Distance from the stream source	km	DSOURCE
Hardness	meq. l^{-1}	HARD
Nitrates-N	mg N-NO_3 l^{-1}	NO_3
Oxygen content	mg l^{-1}	O_2
pH	pH units	pH
Precipitation	mm	PREC
Temperature	°C	TEMP
Integrity metrics		
Composition measures		
Number of Chironomidae taxa	No. of sub-families	CHIR
Number of Ephemeroptera taxa	No. of species	EPH
Number of Plecoptera taxa	No. of species	PLEC
Number of Trichoptera taxa	No. of species	TRIC
Number of EPT taxa	EPH + PLEC + TRIC	EPT
Richness measures		
Total number of taxa	No. of species	TOT
Shannon–Wiener index		H′
Pielou's evenness		E
Tolerance measures		
EPT/(EPT + Chironomidae)		EPT and CHIR

residuals were achieved by using logarithmic transformations ($X' = \log_{10}[X+1]$) in each side of the equation, i.e. on both dependent and independent variables (Zar, 1996). The lack of multicolinearity between independent variables was assured by the inspection of the respective tolerance values.

Since the previous statistical procedures are static, the initial data set included true gradients of environmental characteristics and man-induced disturbances. In this way, the factors of time and space were implicit in the respective treatment and the significant partial regression coefficients were assumed as relevant holistic ecological parameters in the dynamic model construction. This is the heart of the philosophy of the stochastic dynamic model developed. This model does not distinguish between different species within the selected metrics, but considers them as a whole in each corresponding state variable. Therefore, from an holistic perspective, the partial regression coefficients represent the global influence of the environmental variables selected and are of significant importance in several complex ecological processes not included explicitly in the model, but related to the state variables or metrics under consideration. All the modelling procedures were developed using STELLA 5.0®.

For validation purposes, independent biological and physicochemical data from the four sampling stations of the Pinhão watershed (P1, P2, P3 and P4) were used to confront the simulated values of a given metric, resulting from the introduction of the respective real physicochemical data into the model, with the real values of the same metric contemporaneous to those environmental parameters. A regression analysis (Model II) was performed to compare the observed real values of the selected ecological metrics with the expected values obtained by model simulations for the same periods. At the end of each analysis, the 95% confidence limits for the intercept and the slope of the regression line were determined which, together with the results of the respective analysis of variance (ANOVA), allowed us to assess the proximity of the simulations produced with the observed values (Sokal and Rohlf, 1995). When the results of the regression analysis were statistically significant, i.e. when the intercept of the regression line was not statistically different from 0 and the slope was not statistically different from 1, the model simulations were considered validated (Sokal and Rohlf, 1995; Oberdorf et al., 2001).

In order to quantify assessment we must be able to specify the ecological properties that are expected to occur in the absence of human alteration (the pristine condition) or are attainable if human impact ceases. Since we had no knowledge about the biota that existed at the studied sites prior to human alteration, we took the environmental data reported in the eighties as a reference situation. In fact, in that period the studied watersheds presented, in general, good water quality (clean waters, not polluted or little altered), according to the BMWP′ (Alba-Tercedor and Sánchez-Ortega, 1998) and IBB (Pauw and Vanhooren, 1983) indexes.

After the validation process, the model performance was analysed facing scenarios of water quality degradation resulting from organic pollution. Since the sampling station C6, located in the Corgo watershed, was monitored in 1994 for chemical water quality (Sampaio, 1995), approximately 10 years later than the data used for the model construction, this data was used to represent water quality degradation in this site. In fact, according to Sampaio (1995), this sampling station displayed a typical diagnosis of eutrophication. Two scenarios for C6 were considered to evaluate the sensitivity of the developed model in discriminating real perturbations: scenario 1 was assumed, for comparative purposes, as a reference condition (in spite of already not being an unpolluted site) and characterized by the environmental data from 1984 (Cortes, 1992), and scenario 2 was identified as a perturbed condition regarding environmental data from 1994 (Sampaio, 1995). Thereafter, a Mann–Whitney test was performed to compare two different time series from the two scenarios considered.

3. Results

3.1. Effects of environmental factors in biological metrics

A stepwise multiple regression analysis was used to search for significant correlations between the mixed biological metrics and the mixed environmental variables of the three watersheds used in the model construction. Of the 13 environmental variables considered, 4 were excluded from the model ($P > 0.05$), namely chemical oxygen demand, phosphates-P, chlorides, and dissolved oxygen content. The environmen-

Table 2
The regression equations, degrees of freedom (d.f.), coefficient of determination (R^2)

Equations	d.f.	R^2	F
$\log \text{CHIR} = 0.066 + 0.278(\log \text{COND}) - 0.890(\log \text{HARD})$	69	0.181	4.169*
$\log \text{EPH} = 1.805 + 0.255(\log \text{DSOURCE}) - 1.718(\log \text{pH}) - 0.831(\log \text{NO}_3)$	68	0.263	6.637***
$\log \text{PLEC} = -1.385 + 0.145(\log \text{PREC}) + 0.457(\log \text{ALT}) + 0.256(\log \text{DSOURCE})$	68	0.504	19.333***
$\log \text{TRIC} = -0.300 + 0.305(\log \text{BOD}_5) + 0.274(\log \text{ALT}) - 0.822(\log \text{NO}_3)$	68	0.253	6.238***
$\log \text{TOT} = 2.548 + 1.492(\log \text{ALK}) - 1.576(\log \text{pH}) - 0.961(\log \text{NO}_3)$	68	0.206	4.462**
$\log \text{H}' = 0.512 + 0.624(\log \text{ALK}) - 0.093(\log \text{COND})$	68	0.081	3.022*

F-values and their significance level (* $P < 0.05$; ** $P < 0.01$; *** $P < 0.001$) for all the variables combination selected as significant by stepwise multiple regression. The specification of all variable codes is expressed in Table 1.

tal variables associated with a longitudinal gradient seemed to be the main influencing factors on metrics related to those macroinvertebrates more sensitive to organic pollution. In fact, the increase in the number of species of Ephemeroptera and Plecoptera was positively correlated with the distance from stream source (Table 2). Moreover, the number of species of Plecoptera and Trichoptera seemed to be positively influenced by an increase of altitude (Table 2). The increase of nitrate concentrations, an indicator of potential organic perturbation, seemed to negatively affect the total number of taxa, and the Ephemeroptera and Trichoptera compositions (Table 2). The remaining physicochemical significant influences are expressed in Table 2.

3.2. Model conceptualization and equations

The diagram of the model presented in Fig. 2 is based on the relationships detected in multiple regression analysis (Table 2) and on existing relevant regional data sets (Cortes, 1992). Therefore, the model includes the following six state variables: four metrics related to the composition measures of benthic community and two related to their richness measures (Fig. 2). Difference equations that describe the processes affecting the state variables are expressed in a logarithm of composition and richness of the respective biological metrics (Table 3, Difference equations). The initial values of all state variables, indicated in Table 3 (Process equations), were assumed to be zero, given the lack of knowledge of the initial situation in t0. Later, for simulations representation, the initial value was discarded, since only in t1 (first month of the simulation) was it possible to take into account the influences of the environmental variables, whose seasonal fluctuations were introduced into the model as table functions (Table 3, Table functions).

The inflows affecting the ecological metrics state variables, Chironomidae (Chir gains), Ephemeroptera (Eph gains), Plecoptera (Plec gains), Trichoptera (Tric gains), total number of taxa (Tot gains), and Shannon–Wiener index (H′ gains), were based on the positive constants and all positive partial coefficients of each metric resulting from the previous multiple regression analysis (Fig. 2, Tables 2 and 3, Difference and Process equations). However, all metrics were affected by an outflow (Chir losses, Eph losses, Plec losses, Tric losses, Tot losses, H′ losses) related to the negative constants and partial regression coefficients (Fig. 2, Tables 2 and 3, Difference and Process equations). Although the composition and richness output for each metric in our stochastic dynamic model simulation is composed of a given value per time unit, the respective state variable may result in a cumulative behaviour over time in response to environmental condition changes. Therefore, to prevent this from happening, six outflow adjustments were incorporated into the model (Chir adjust, Eph adjust, Plec adjust, Tric adjust, Tot adjust, and H′ adjust). These outflow adjustments aim to empty the ecological metric state variables at each time step, by a "flushing cistern mechanism", before beginning the next step with new environmental influences (Fig. 2 and Table 3, Difference and Process equations). For process compatibilities and a more realistic comprehension of the model simulations, some conversions were introduced, denominated as associated variables (Fig. 2 and Table 3, associated variables). Regarding the biological metrics, these conversions were obtained through an inverse transformation (anti-logarithmic), which transforms logarithms into composition and

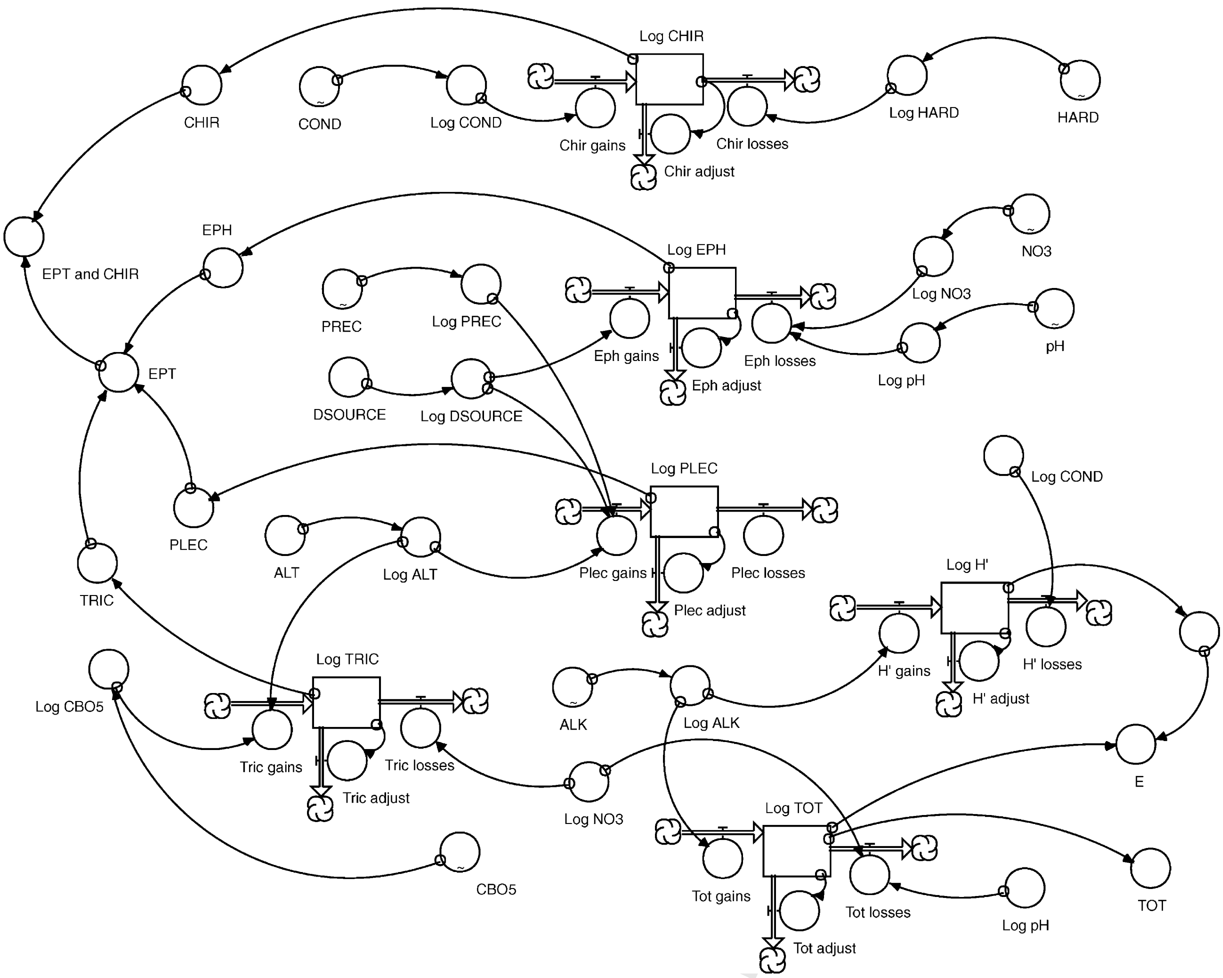

Fig. 2. Conceptual diagram of the model used to predict biological metrics by given environmental variables from the studied watersheds in Northeast Portugal. The specification of all variable codes is expressed in Table 1.

richness expressed in the original measurement units (CHIR, EPH, PLEC, TRIC, TOT, and H′). The physicochemical variables were logarithm transformed for a compatible integration into the balance of the state variables (Fig. 2 and Table 3, associated variables). This transformation was incorporated because the data required for the state variables balances should use the same units to obtain the significant partial regression coefficients, assumed to be holistic ecological parameters (see Section 2). Therefore, only logarithms of the physicochemical variables are acceptable in the inflows and outflows of the state variables (Fig. 2 and Table 3, Difference and Process equations). Thus, the model is ready to receive and transform real data from the environmental variables and convert logarithmic outputs from state variables simulations into original units. Other variables, resulting from simple mathematical operations between the associated variables, such as Pielou's evenness (E), the ratio EPT/(EPT + Chironomidae) (EPT and CHIR), and the EPT metric (EPT), were used to complete the output of the model and named composed variables (Table 3, composed variables). Some environmental values, such as altitude (ALT) and distance from the stream source (DSOURCE), were static, with no variation during the simulated period, and,

Table 3
Mathematical equations used in Stella for the relationships between the composition, richness and tolerance metrics and the environmental physicochemical variables from the studied watersheds

Difference equations

$\log \mathrm{CHIR}(t) = \log \mathrm{CHIR}(t - \mathrm{d}t) + (\text{Chir gains} - \text{Chir losses} - \text{Chir adjust})\mathrm{d}t$

$\log \mathrm{EPH}(t) = \log \mathrm{EPH}(t - \mathrm{d}t) + (\text{Eph gains} - \text{Eph losses} - \text{Eph adjust})\mathrm{d}t$

$\log \mathrm{PLEC}(t) = \log \mathrm{PLEC}(t - \mathrm{d}t) + (\text{Plec gains} - \text{Plec losses} - \text{Plec adjust})\mathrm{d}t$

$\log \mathrm{TRIC}(t) = \log \mathrm{TRIC}(t - \mathrm{d}t) + (\text{Tric gains} - \text{Tric losses} - \text{Tric adjust})\mathrm{d}t$

$\log \mathrm{TOT}(t) = \log \mathrm{TOT}(t-\mathrm{d}t) + (\text{Tot gains} - \text{Tot losses} - \text{Tot adjust})\mathrm{d}t$

$\log \mathrm{H}'(t) = \log \mathrm{H}'(t - \mathrm{d}t) + (\mathrm{H}' \text{ gains} - \mathrm{H}' \text{ losses} - \mathrm{H}' \text{ adjust})\mathrm{d}t$

Process equations

(a) Chironomidae

Initial richness of $\log \mathrm{CHIR} = 0$

Chir gains $= 0.066 + 0.278 \log \mathrm{COND}$

Chir losses $= 0.890 \log \mathrm{HARD}$

Chir adjust $= \log \mathrm{CHIR}$

(b) Ephemeroptera

Initial richness of $\log \mathrm{EPH} = 0$

Eph gains $= 1.805 + 0.255 \log \mathrm{DSOURCE}$

Eph losses $= 1.718 \log \mathrm{pH} + 0.831 \log \mathrm{NO_3}$

Eph adjust $= \log \mathrm{EPH}$

(c) Plecoptera

Initial richness of $\log \mathrm{PLEC} = 0$

Plec gains $= 0.145 \log \mathrm{PREC} + 0.457 \log \mathrm{ALT} + 0.256 \log \mathrm{DSOURCE}$

Plec losses $= 1.385$

Plec adjust $= \log \mathrm{PLEC}$

(d) Trichoptera

Initial richness of $\log \mathrm{TRIC} = 0$

Tric gains $= 0.305 \log \mathrm{CBO_5} + 0.274 \log \mathrm{ALT}$

Tric losses $= 0.300 + 0.822 \log \mathrm{NO_3}$

Tric adjust $= \log \mathrm{TRIC}$

(e) Total number of taxa

Initial richness of $\log \mathrm{TOT} = 0$

Tot gains $= 2.548 + 1.492 \log \mathrm{ALK}$

Tot losses $= 1.576 \log \mathrm{pH} + 0.961 \log \mathrm{NO_3}$

Tot adjust $= \log \mathrm{TOT}$

(f) Shannon–Wiener index

Initial richness of $\log \mathrm{H}' = 0$

H' gains $= 2.548 + 1.492 \log \mathrm{ALK}$

H' losses $= 1.576 \log \mathrm{pH} + 0.961 \log \mathrm{NO_3}$

H' adjust $= \log \mathrm{H}'$

Associated variables

$\mathrm{CHIR} = 10\hat{}(\log \mathrm{CHIR}) - 1$

$\mathrm{EPH} = 10\hat{}(\log \mathrm{EPH}) - 1$

$\mathrm{PLEC} = 10\hat{}(\log \mathrm{PLEC}) - 1$

$\mathrm{TRIC} = 10\hat{}(\log \mathrm{TRIC}) - 1$

$\mathrm{TOT} = 10\hat{}(\log \mathrm{TOT}) - 1$

$\mathrm{H}' = 10\hat{}(\log \mathrm{H}') - 1$

$\log \mathrm{ALK} = \log_{10} (\mathrm{ALK} + 1)$

$\log \mathrm{ALT} = \log_{10} (\mathrm{ALT} + 1)$

$\log \mathrm{BOD_5} = \log_{10} (\mathrm{BOD_5} + 1)$

$\log \mathrm{COND} = \log_{10} (\mathrm{COND} + 1)$

$\log \mathrm{DSOURCE} = \log_{10} (\mathrm{DSOURCE} + 1)$

$\log \mathrm{HARD} = \log_{10} (\mathrm{HARD} + 1)$

$\log \mathrm{NO_3} = \log_{10} (\mathrm{NO_3} + 1)$

$\log \mathrm{O_2} = \log_{10} (\mathrm{O_2} + 1)$

Table 3 (*Continued*)

$\log pH = \log_{10}(pH + 1)$
$\log PPREC = \log_{10}(PREC + 1)$

Composed variables
$E = H'/\log TOT$
$EPT = EPH + PLEC + TRIC$
$EPT\ and\ CHIR = EPT/(CHIR + EPT)$

Environmental constants
$ALT = 690$
$DSOURCE = 7.5$

Table functions
ALK = Graph (month, meq. l^{-1})
(0.00, 0.18), (1.09, 0.18), (2.18, 0.18), (3.27, 0.2), (4.36, 0.2), (5.45, 0.2), (6.55, 0.26), (7.64, 0.26), (8.73, 0.26), (9.82, 0.13), (10.9, 0.13), (12.0, 0.13)
BDO_5 = Graph (month, mg $O_2\ l^{-1}$)
(0.00, 0.42), (1.09, 0.42), (2.18, 0.42), (3.27, 0.63), (4.36, 0.63), (5.45, 0.63), (6.55, 2.40), (7.64, 2.40), (8.73, 2.40), (9.82, 1.70), (10.9, 1.70), (12.0, 1.70)
COND = Graph (month, μmhos cm^{-1})
(0.00, 33.3), (1.09, 33.3), (2.18, 33.3), (3.27, 33.5), (4.36, 33.5), (5.45, 33.5), (6.55, 48.0), (7.64, 48.0), (8.73, 48.0), (9.82, 37.6), (10.9, 37.6), (12.0, 37.6)
HARD = Graph (month, meq. l^{-1})
(0.00, 0.19), (1.09, 0.19), (2.18, 0.19), (3.27, 0.23), (4.36, 0.23), (5.45, 0.23), (6.55, 0.1), (7.64, 0.1), (8.73, 0.1), (9.82, 0.3), (10.9, 0.3), (12.0, 0.3)
NO_3 = Graph (month, mg N-$NO_3^-\ l^{-1}$)
(0.00, 0.01), (1.09, 0.01), (2.18, 0.01), (3.27, 0.00), (4.36, 0.00), (5.45, 0.00), (6.55, 0.03), (7.64, 0.03), (8.73, 0.03), (9.82, 0.13), (10.9, 0.13), (12.0, 0.13)
O_2 = Graph (month, mg l^{-1})
(0.00, 9.17), (1.09, 9.17), (2.18, 9.17), (3.27, 9.10), (4.36, 9.10), (5.45, 9.10), (6.55, 7.60), (7.64, 7.60), (8.73, 7.60), (9.82, 10.2), (10.9, 10.2), (12.0, 10.2)
pH = Graph (month, pH units)
(0.00, 6.29), (1.09, 6.29), (2.18, 6.29), (3.27, 6.40), (4.36, 6.40), (5.45, 6.40), (6.55, 6.50), (7.64, 6.50), (8.73, 6.50), (9.82, 6.30), (10.9, 6.30), (12.0, 6.30)
PREC = Graph (month, mm)
(0.00, 80.4), (1.09, 80.4), (2.18, 80.4), (3.27, 22.7), (4.36, 22.7), (5.45, 22.7), (6.55, 137), (7.64, 137), (8.73, 137), (9.82, 154), (10.9, 154), (12.0, 154)

As an example, the environmental data of the sampling station P1 was used. The specification of all variable codes is expressed in Table 1.

therefore, were introduced as environmental constants (Table 3, Environmental constants).

3.3. Model simulations

The temporal unit chosen was the month, because it represents the average ecological variations that occur in lotic systems throughout one or several years. The Euler's integration method was used. For precipitation values, we considered the data from a typical year that would correspond to the averages calculated over a period of 30 years (1961–1990). In this work, all the performed simulations have a total length of 12 months, beginning in the spring, coinciding with the first sampling campaign carried out by Cortes (1992).

For the majority of the relevant metrics adopted, the model successfully predicts the behaviour of the biological metrics under the influence of independent environmental variables from the Pinhão watershed sampling stations (P1, P2, P3 and P4) (Table 4). With the exception of P3, all the simulations were statistically validated by the regression analysis (Model II) of the remaining sampling stations (Table 4). Fig. 3 illustrates the confrontation between simulated and real values for the most revealing metrics under consideration (Chironomidae, EPT, number of total taxa, and Shannon–Wiener index). For these metrics, the model simulations accurately predicted the real values for P1, P2 and P4, with generally the same behavioural tendencies, but not for P3 (Fig. 3 and Table 4). In fact,

Table 4
Regression analysis (Model II) intercepts and slopes, and the respective 95% confidence limits (in parenthesis), degrees of freedom (d.f.), coefficient of determination (R^2)

Metrics	Site	Intercept	Slope	d.f.	R^2	F
EPH	P1	−0.45 (−1.05; 0.03)	1.21 (1.02; 1.45)	11	0.936	161.13***
	P2	0.06 (−1.10; 0.88)	1.17 (0.87; 1.60)	11	0.831	54.211***
	P3	−0.056 (−0.83; 0.52)	0.86 (0.59; 1.21)	11	0.788	40.92***
PLEC	P1	−0.73 (−1.24; −0.32)	1.43 (1.20; 1.72)	11	0.933	154.27***
	P2	−0.029 (−0.20; 0.13)	0.69 (0.57; 0.80)	11	0.941	176.56***
	P3	−2.80 (−119.12; −0.41)	3.65 (1.73; 96.76)	11	0.307	4.86*
	P4	−0.003 (−0.31; 0.23)	1.12 (0.82; 1.55)	11	0.819	49.68***
TRIC	P1	−0.69 (−2.67; 0.55)	1.55 (1.14; 2.21)	11	0.810	46.77***
	P2	−0.25 (−2.58; 1.02)	1.49 (1.04; 2.41)	11	0.716	27.77***
	P3	−1.9 (−11.43; 0.64)	2.71 (1.58; 6.94)	11	0.515	11.69**
	P4	0.36 (−0.26; 0.85)	1.14 (−1.41; 0.92)	11	0.907	107.69***
EPT	P1	−2.05 (−4.43; −0.23)	1.43 (1.18; 1.75)	11	0.920	126.36***
	P2	0.45 (−1.60; 2.02)	1.09 (0.85; 1.39)	11	0.883	83.41***
	P3	−3.42	1.92	11	0.235	3.37 (n.s.)
	P4	−0.11 (−1.54; 1.01)	1.10 (0.89; 1.38)	11	0.901	99.89***
CHIR	P1	−0.24 (−2.55; 0.56)	1.76 (0.99; 3.94)	11	0.732	12.69**
	P2	−0.42 (−4.74; 0.83)	1.45 (0.69; 4.06)	11	0.434	8.44*
	P3	−1.04 (−7.52; 0.44)	1.39 (0.58; 4.97)	11	0.370	6.46*
	P4	−0.49 (−3.59; 0.61)	1.16 (0.51; 2.97)	11	0.431	8.34*
EPT and CHIR	P1	−0.008 (−0.09; 0.06)	1.12 (1.01; 1.22)	11	0.981	570.69***
	P2	0.015 (−0.11; 0.12)	1.05 (0.89; 1.22)	11	0.948	202.19***
	P3	0.014 (−0.12; 0.13)	1.09 (0.93; 1.29)	11	0.944	184.27***
	P4	−0.03 (−0.24; 0.13)	1.12 (0.88; 1.43)	11	0.977	468.98***
TOT	P1	−2.44 (−8.07; 1.81)	1.08 (0.83; 1.40)	11	0.868	72.49***
	P2	−0.108 (−0.83; 0.58)	1.08 (1.04; 1.13)	11	0.996	2807.2***
	P3	−13.85	1.91	11	0.254	3.75 (n.s.)
	P4	−0.89 (−4.59; 2.04)	0.93 (0.73; 1.20)	11	0.878	79.05***
H′	P1	−0.026 (−0.17; 0.11)	1.08 (0.98; 1.18)	11	0.982	595.02***
	P2	−0.19 (−0.89; 0.27)	1.34 (0.99; 1.87)	11	0.820	50.19***
	P3	−0.56 (−2.67; 0.30)	1.59 (0.93; 3.23)	11	0.575	14.91**
	P4	−0.37 (−1.45; 0.23)	1.25 (0.79; 2.09)	11	0.674	22.70***
E	P1	−0.033 (−0.15; 0.06)	1.18 (0.99; 1.41)	11	0.935	154.38***
	P2	−0.07 (−0.35; 0.10)	1.32 (0.94; 1.92)	11	0.787	40.76***
	P3	−0.089 (−0.84; 0.19)	1.32 (0.68; 2.98)	11	0.499	10.96**
	P4	−0.15 (−0.53; 0.06)	1.35 (0.89; 2.13)	11	0.717	27.94***

F-values and significance level ($^{*}P < 0.05$; $^{**}P < 0.01$; $^{***}P < 0.001$), for all the observed vs. expected values of the biological metrics. P1, P2, P3 and P4 represent the four sampling stations of the Pinhão river. (n.s.) not significant. The specification of all variables codes is expressed in Table 1.

the worst performances of the model were always obtained in the sampling station P3, located in an atypical tributary of the Pinhão river (Fig. 1). In P3, the simulated values were frequently underestimated or overestimated (Fig. 3 and Table 4), probably because, in this case, the environmental variables selected do not capture all the relevant variability and heterogeneity of this particular site. Overall, for the majority of the simulations, the model behaves as expected for the reference situation considered.

After the validation procedures, we tested the model's performance in the face of a new scenario of eutrophization in the sampling station C6, from the Corgo river. Using the same illustrative criteria used

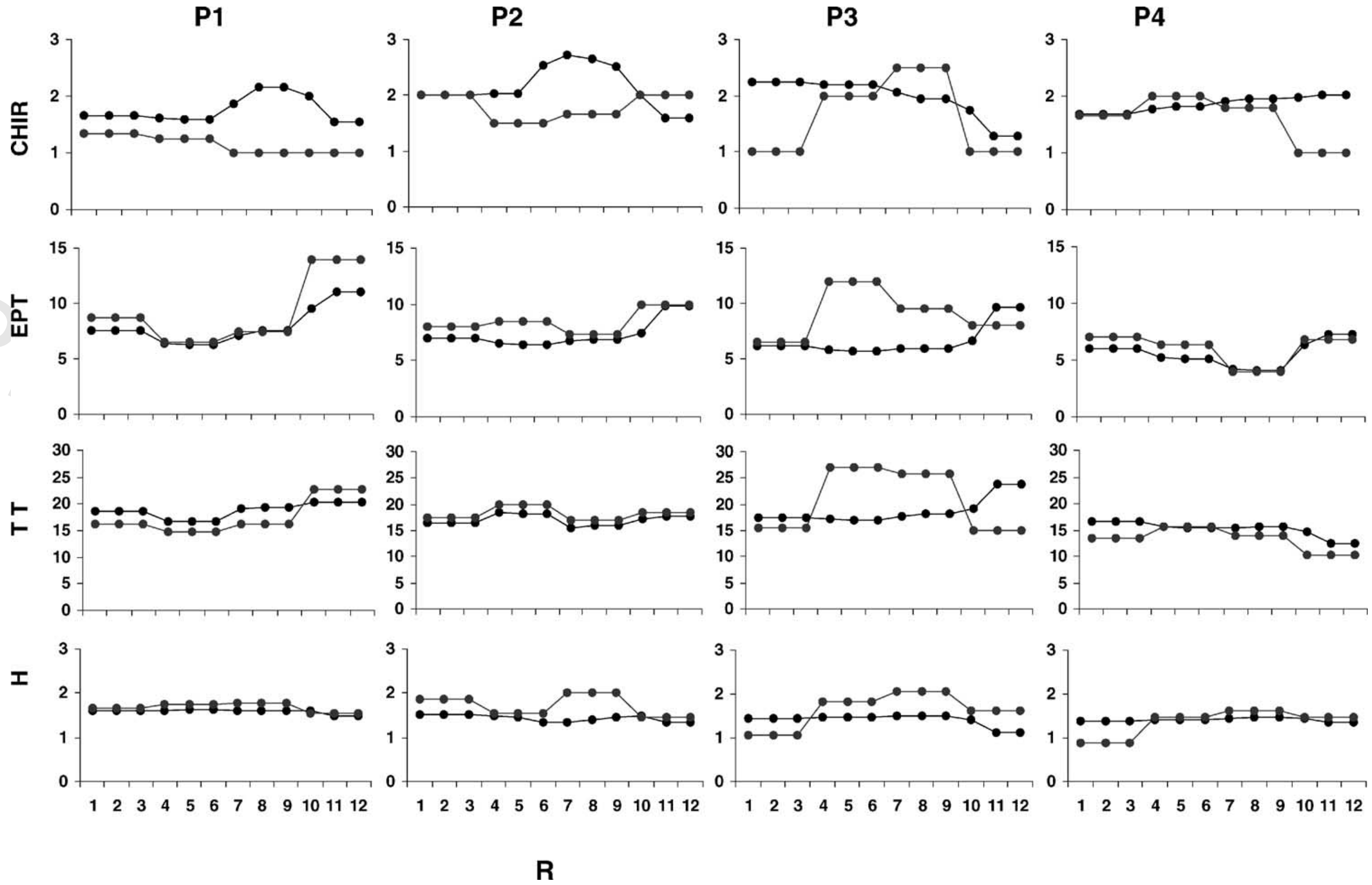

Fig. 3. Graphical comparisons between expected (black lines) and observed (grey lines) values of the following biological metrics: Chironomidae (CHIR), EPT, total number of taxa (TOT) and Shannon–Wiener index (H′). P1, P2, P3 and P4 are the four sampling stations of the Pinhão watershed.

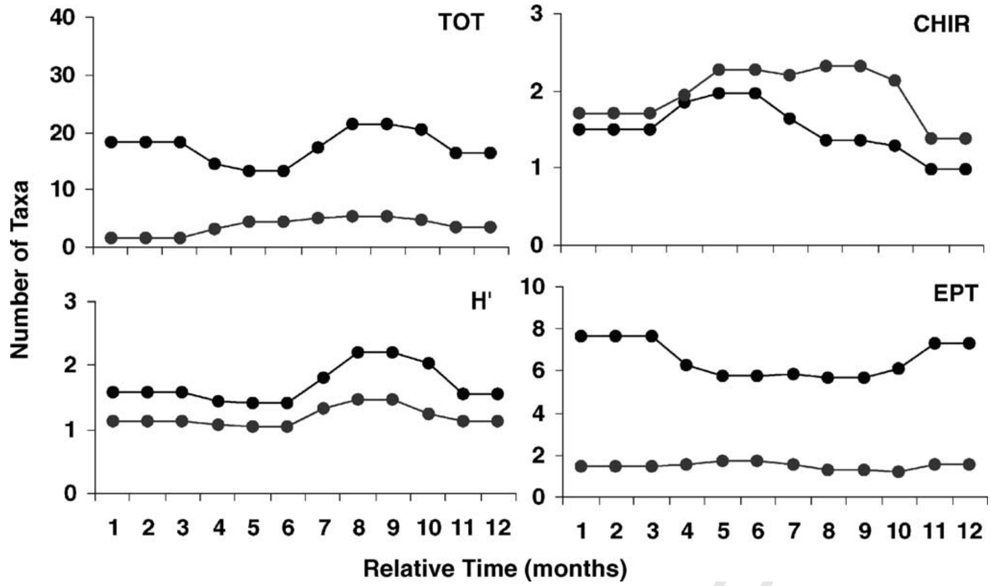

Fig. 4. Model simulations for Chironomidae (CHIR), EPT, total number of taxa (TOT) and Shannon–Wiener index (H′) facing two different scenarios: scenario 1, the reference condition in 1985 (black line) and scenario 2, the perturbed condition in 1995 (grey line), both from the sampling station C6 of the Pinhão watershed.

in Fig. 3, the comparisons between the simulated values of the four more revealing metrics, obtained from scenario 1 (reference condition in 1984) and from scenario 2 (organic degradation in 1994) are shown in Fig. 4. The model reacted to the new scenario in a differentiated way. In fact, a clear decrease in the composition and richness of the metrics more sensitive to organic pollution was evident when water quality declined in the scenario 2 (Fig. 4). On the contrary, the number of Chironomidae taxa, well adapted to the organic degradation, increased in scenario 2 (Fig. 4). These results were statistically corroborated by the Mann–Whitney test that indicated an expected discrimination between scenario 1 and scenario 2, regarding the decreases in EPT ($U = 144$, $n = 24$, $P < 0.001$), total number of taxa ($U = 144$, $n = 24$, $P < 0.001$) and Shannon–Wiener index values ($U = 138$, $n = 24$, $P < 0.001$), and the increase of Chironomidae taxa ($U = 144$, $n = 24$, $P < 0.001$).

4. Discussion

The stochastic-dynamic methodology developed in this study seems to represent a useful contribution to the assessment of the ecological status of typical running waters, predicting the structure and diversity of key aquatic biological metrics. In fact, the simulation results showed that the biological metrics selected as state variables were not indifferent to changes in the environmental conditions, namely when sites relatively unaffected by human activities were changed by man-induced disturbances, such as organic pollution. The relevant ecological drifts observed are in agreement with other studies that have investigated the biological consequences of aquatic ecosystem changes by these type of anthropogenic impacts on key aquatic communities in general and on macroinvertebrates in particular (e.g. Cortes, 1992; Wright et al., 1995; Fore et al., 1996; Hutchens et al., 1998; DeWalt et al., 1999; Davies et al., 2000; Whiles et al., 2000; Karr and Rossano, 2001; Karr, 2002).

Since the attributes of the macroinvertebrate community structure, such as their respective composition, diversity and abundance are influenced by certain environmental conditions (Karr and Dudley, 1981; Norris et al., 1995; Richards et al., 1993; Roth et al., 1996; Townsend et al., 1997a,b; Lounaci et al., 2000; Li et al., 2001), the developed methodology can be used as a predictive tool for running waters ecological assessment. Another goal when developing methods for assessing changes in the ecological integrity of an aquatic ecosystem is the feasibility of application and extent to which the results can be reproduced in other areas (Andreasen et al., 2001). The methodology proposed is expeditious and easily applicable to other aquatic ecosystems affected by environmental changes. The above multivariate statistical analysis used gave robustness to the dynamic interactions, with holistic and ecological relevance included in the model construction and reduces the number of pre-conceptions added to the model. Nevertheless, if we consider that validation is a fundamental process to test the relative accuracy of the model response in relation to its applicability (Rykiel, 1996) then two main questions remain within the present methodology. The first deals with the need for a validation carried out over a wider geographical area (Karr, 2002) and the second requires the use of other key aquatic communities, such as phytoplankton, microphytobenthos, macrophytes, and fish (Barbour et al., 1999).

Despite these considerations, the philosophy of this stochastic-dynamic methodology can be applicable to aquatic ecosystem management and policymaking, providing a useful contribution to define the reference conditions for surface water bodies from the quality elements specified in point 1.1 in Annex V of the Water Framework Directive 2000/60/EC. This will help not only the public end-users, but also those evaluating environmental quality.

Overall, the main results showed that, as with any complex process in science, it is valid, interesting, and instructive to construct stochastic dynamic models focusing on the interactions between key-components of changing natural ecosystems. This approach may also provide a useful starting point from which to develop more global techniques in the scope of this research area, such the spatial dynamic models and to create expeditious interfaces with Geographical Information Systems, which will make the methodology more instructive and credible to decision-makers and environmental managers (Costanza, 1992, Santos and Cabral, submitted).

Uncited references

Jørgensen (1999) and Shannon and Wiener (1963).

Acknowledgements

Thanks to Audrey Gerry for the English revision of the manuscript and to Ana Sampaio, from the Biological and Environmental Engineering Department of the University of Trás-os-Montes e Alto Douro, who recorded the physicochemical parameters from the Corgo river in 1994.

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