EPJ Web of Conferences **269**, 01051 (2022) https://doi.org/10.1051/epjconf/202226901051
EFM 2019

Using the AQUATOX model to forecast water bodies quality status response to environmental perturbations

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Abstract. In the last decades, the scientific community has developed many methods and approaches for the assessment of surface waters quality status and the relative impacts of anthropogenic pressures including, among the others, municipal and industrial wastewater treatment plants, agriculture, animal farming and many other land uses. According to the Water Framework Directive (WFD; 2000/60/EC), each EU Member State has been committed to identifying River Basin Districts, in which, ideally, every water body within European boundaries should have been included. As a contribution to the quality assessment of the Sardinian River Basin District, in the framework of the project "Hydraulic and environmental modelling for the gap analysis and the identification of programmes of measures aimed to satisfy the environmental quality objectives" funded by the Regione Sardegna, we applied a simplified version of the AQUATOX model, developed for investigating its feasibility and validity in case of missing or poor input data and information, on the river Cixerri case study.

1 Introduction

As discussed in previous study on the topic presented, "Validation of a simplified AQUATOX model to assess quality status of a model river in Sardinia", AQUATOX validation can be a difficult task when is applied to the Mediterranean contexts. Such difficulties derived mainly from its large amount of data required, that implies strong differentiations between locations. However, from that study some general conclusions can be drawn, and some similar applications with good results can be found in the literature (1). So, in next sections is shown how including more ecosystem components leads to a more realistic output of AQUATOX model, encouraging its use for water bodies responses to pressures and stressors forecasting.

As a brief description of the main reasons why AQUATOX was chosen, in Table 1, a summary of the comparison with other models is reported, from (2). AQUATOX is perhaps the most complete ecological risk simulation model, and it can be used for different purposes. Initially, it has been created for studying the United States water bodies, but rapidly it has been used also in numerous different countries. For instance, in (3) a study on the Songhua river is presented, related to the accidental discharge of nitrobenzene on November 2005: the model has been used for simulating the nitrobenzene distribution with respect to time, and for determining the potential ecological impact.

Assessing water bodies quality, according to 2000/60/EC directive, means to give a judgement basing on a set of evaluated parameters for that water body, namely biological indicators, morphological status, chemical-physical condition, and chemical pollutants presence.

Table 1. The comparison of AQUATOX and other available models, in terms of variables and processes considered.

State variables and processes	AQUATOX	CATS	CASM	Qual2K	WASP7	EFDC-HEM3D	QEAFdChn	BASS	QSim
Nutrients	X	X	X	X	X	X			X
Sediment diagenesis	X			X	X	X			
Detritus	X	X	X	X	X	X			X
Dissolved oxygen	X		X	X	X	X			X
DO effects on biota	X								X
pH	X			X					X
NH_4 toxicity	X								
Sand/silt/clay	X				X	X			
Sediment effects	X								
Hydraulics						X			X
Heat budget				X	X	X			X
Salinity	X				X	X			
Phytoplankton	X	X	X	X	X	X			X
Periphyton	X	X	X	X	X				X
Macrophytes	X	X	X						X
Zooplankton	X	X	X						X
Zoobenthos	X	X	X						X
Fish	X	X	X					X	X
Bacteria			X						X
Pathogens				X		X			
Organic toxicant fate	X	X			X			X	
Organic toxicants in									
Sediments	X	X			X	X			
Stratified sediments	X				X	X			
Phytoplankton	X	X							
Periphyton	X	X							
Macrophytes	X	X							
Zooplankton	X	X					X		
Zoobenthos	X	X					X		
Fish	X	X					X	X	
Birds or other animals	X	X							
Ecotoxicity	X	X	X					X	
Linked segments	X			X	X	X	X		X

Quality judgement can be expressed basing on indications from D.Lgs. 152/2006, and general method for the ecological state determination, available in several Italian Agenzia Regionale Protezione Ambiente (ARPA) websites (e.g. ARPA Lombardia). Final ecological status depends on the combination of the four aforementioned factors, one of which is called the LIMeco parameter (five levels, Level 1 is the best, Level

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5 is the worst), represents the chemical-physical status of the water body and involves dissolved oxygen, ammonia, nitrate and phosphorus concentration values.

2 Case study

In "Validation of a simplified AQUATOX model to assess quality status of a model river in Sardinia", the Cixerri river was considered as the case study. Here, only a part of the Cixerri river has been investigated: the considered branch has a slope of roughly 23% and a length of 30 km.

Fig. 1. Satellite framing of the investigated trait of Cixerri river with GIS data used.

The satellite framing with the vector data of the Geographic Information System (GIS) used for the study case is shown in Fig. 1 (the free software QGIS was used). Available monitoring data on the Cixerri river were used both to increment the input dataset and to improve the description of the site in order to better compare model results with real observed prospect. The configuration related to the case study of the Blue Earth River has been set as initial in the current model, available in AQUATOX dataset: it is a practice suggested by AQUATOX developers (2), instead of building a simulation starting from zero. This is because the model needs to have every parameter available for the implementation of equations, and for certain cases, rough information is better than no information at all. For the flow rate values, it has been considered the monthly average value, extracted by the most recent public study for the river considered in this case study.

3 Results and discussion

For the model validation, in this study another specification has been included: considering the data of Blue Earth River as described in case study section, algae species presence and the food web, have been modified as suggested in (1) for the Po river. This study case was chosen also since it represents a Mediterranean case study, and it allows to get a more realistic representation of what happens in terms of predator-prey mechanism in a Sardinian river. In Fig. 2, the proposed schematisation is shown.

Table 2 shows the complete set of initial conditions for chemical-physical parameters and some related to algae life-cycle.

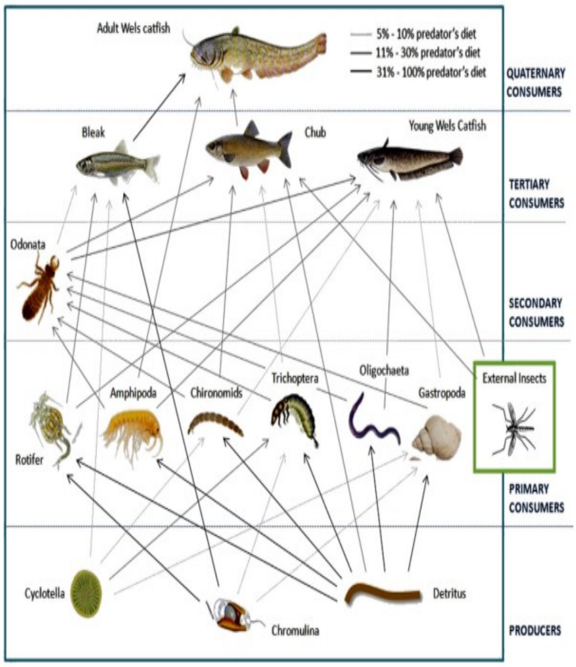

Fig. 2. Food web schematisation for a Mediterranean river (Grechi et al., 2016).

Table 2. Initial conditions for algae (Grechi et al., 2016).

Category	Microalgae	
Default organism/group in the AQUATOX plant library	*Cyclotella*	*Isochryses*
Po river compartment (and abbreviation)	*Cyclotella (Cy)*	*Chromulina (Chro)*
Initial biomass (mg dry/L)	0.12	0.0296
Loading from upstream	Calculated using the AQUATOX option "Enhanced Phytoplankton Retention"	Calculated using the AQUATOX option "Enhanced Phytoplankton Retention"
Saturating light (Ly/d)	22.5	67
P half-saturation (mg/l)	0.05	0.046
N half-saturation (mg/l)	0.117	0.006
Inorg. C half-saturation (mg/l)	0.054	0.054

Category	Microalgae	
Default organism/group in the AQUATOX plant library	*Cyclotella*	*Isochryses*
Po river compartment (and abbreviation)	*Cyclotella (Cy)*	*Chromulina (Chro)*
Temp. response slope	1.8	1.8
Optimum temperature (°C)	23.5	20
Maximum temperature (°C)	30	35
Min. adaptation temperature (°C)	7	2
Max. photosynthetic rate (1/d)	1.87	2
Photorespiration coefficient (1/d)	0.026	0.026
Respiration rate at 20 °C ($g/(g\ d)^{-1}$)	0.0752	0.0483
Mortality coefficient ($g/(g\ d)^{-1}$)	0.001	0.009
Exponential mortality coefficient ($g/(g\ d)^{-1}$)	0.01	0.01
Light extinction	0.02	0.01
Wet to dry mass	5	5
Lipid fraction (kg_{lipid} kg^{-1} wet body)	0.005	0.005

In the following paragraph, a discussion about simulations. As highlighted in Section 3, in this study, the aim was, first, to underline model sensitivity to algae good representation (as the algae species presence and the food web have been modified, as suggested in (1), for the Po river), and secondly to use the model to evaluate the Cixerri water body status. The main morphological data used were:

- River length;
- River mean surface;
- Initial water volume;
- Mean depth;
- Mean slope;
- Input and output water flows;
- Initial total nitrogen concentration;
- Initial total phosphorus concentration;
- Nitrogen and phosphorus discharges.

This type of data is available in the "Piano Stralcio Fasce Fluviali" (PSFF) of Regione Sardegna website. Nitrogen and phosphorus discharges are meant to be both punctual and diffuse pressures, even if in simulations differentiation between these two cases has been made.

Three different types of simulation have been conducted: "Whole", "Parted 1" and "Parted 2". "Whole" simulation is the first, and starts on 01/01/2011, ending on 31/12/2016, this period was chosen based on nutrients data on tap. Initial values for nitrogen and phosphorus concentrations were the average of first year values. "Parted 1" is actually a simulation series, in which the total lapse is divided into sub-periods with one-year duration (five simulations). The first simulation has for N and P input values those observed at the upstream monitoring station in the first part of the monitoring period of 2011. The second receives the output of the first, and so on up to the fifth. It is worth to underline that, even if nitrogen and phosphorus concentrations were taken from precedent simulation output, the other parameters (e.g. algae species and their concentrations) return to initial values once re-starting simulations (an attempt to neglect simulation effects on those parameters, investigating only on nutrients fate). "Parted 2" carries the same scheme as "Parted 1", but with every re-starting of the simulation, input data for N and P is the average of the observed values for the first part of the monitoring period in the respective year. The first simulation received average data registered in the first part of monitoring period in 2011, the second average data registered in the first part of 2012, and so on, up to the fifth simulation.

In following tables the results of Cixerri simulation are reported: Fig. 3, Table 3 and Fig. 4,

Table 4 for total nitrogen and phosphorus concentration, respectively, considering only punctual pressures and neglecting diffuses; Fig. 5, Table 5 and Fig. 6,

Table 6 for nitrogen and phosphorus, respectively, considering all pressures in the water body.

In general, it can be difficult to determine the best method: in most cases, and considering total duration averaged results, "Par 2" method seems to show a better correspondence with observed data, comparing single-year averaged concentrations, but it is not ever true (e.g. for year 2014 of Fig. 5); a decreasing accuracy from 2011 to 2016 can be detected in the "Whole" simulations (for instance in Fig. 3). Considering diffuse pressure improves model performance more in reference to phosphorus rather than to nitrogen.

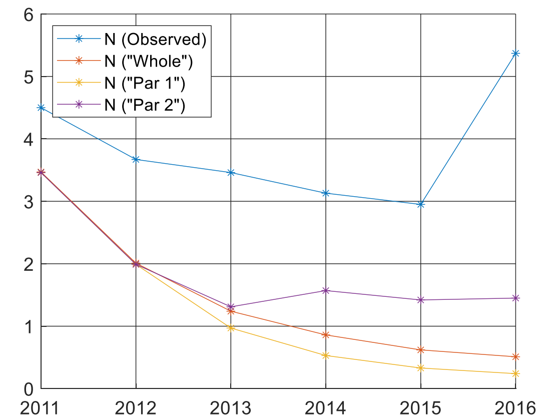

Fig. 3. Comparison between model results and observed concentrations, yearly averaged values (total nitrogen).

Table 3. Total Nitrogen results from model simulation, considering only punctual pressures (total simulation duration average).

N (Observed)	N (“Whole”)	N (“Par 1”)	N (“Par 2”)
3.54	1.47	1.26	1.87

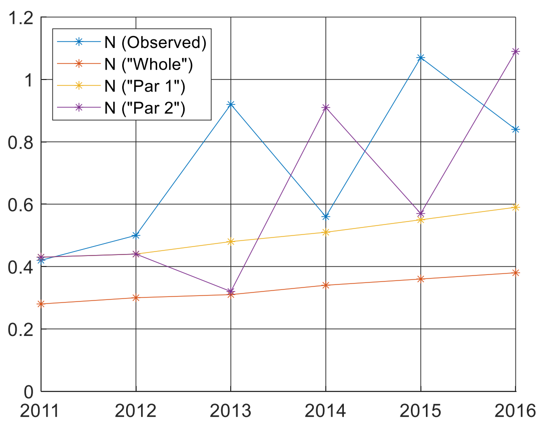

Fig. 4. Comparison between model results and observed concentrations, yearly averaged values (phosphorus).

Table 4. Phosphorus results from model simulation, considering only punctual pressures (total simulation duration average).

Year	P (Observed)	P (“Whole”)	P (“Par 1”)	P (“Par 2”)
Total duration	0.70	0.33	0.50	0.63

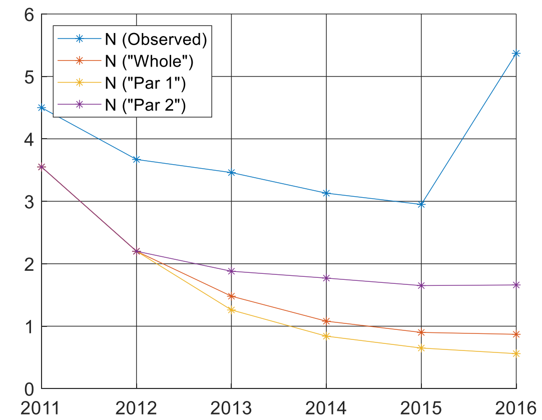

Fig. 5. Comparison between model results and observed concentrations, yearly averaged values (total nitrogen).

Table 5. Total Nitrogen results from model simulation, considering all pressures (total simulation duration average).

Year	N (Observed)	N (“Whole”)	N (“Par 1”)	N (“Par 2”)
Total duration	3.54	1.68	1.51	2.11

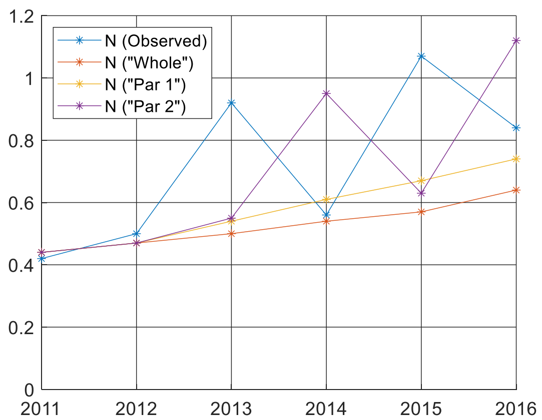

Fig. 6. Comparison between model results and observed concentrations, yearly averaged values (phosphorus).

Table 6. Total Phosphorus results from model simulation, considering all pressures (total simulation duration average).

Year	P (Observed)	P (“Whole”)	P (“Par 1”)	P (“Par 2”)
Total duration	0.70	0.53	0.58	0.70

According to the examined period, considering oxygen data in Cixerri water body, and involving simulation outputs in terms of nutrients concentration, it is possible to estimate the water body environmental quality, in terms of LIMeco, for the considered years, and in relation with different types of simulation.

Table 7. LIMeco levels for the case study, comparison between observations and simulation results.

Year	(Observed)	(“Whole”)	(“Par 1”)	(“Par 2”)
2011	Level 4	Level 4	Level 4	Level 4
2012	Level 4	Level 4	Level 4	Level 4
2013	Level 4	Level 4	Level 4	Level 4
2014	Level 4	Level 3	Level 3	Level 4
2015	Level 4	Level 3	Level 3	Level 4
2016	Level 4	Level 3	Level 2	Level 4

As shown in Table 7, except for the last year of “Par 1” simulation, in which underestimation of concentrations seems to be too relevant, there is a good agreement between monitoring-derived judgement and simulation output-derived judgement. As described above, this is an important fact in view to use forecast modelling to make decisions about measures to take in a certain water body.

4 Conclusions

One of the main results of this study is the obtaining of better accuracy of the model when implementing the ecosystem components: AQUATOX simulates the whole eco-process, and it is not supposed to be used to reproduce nutrients transportation and transformation without a certain accuracy degree in characterizing the ecological component of the river, vegetation and animals. This could be noticed comparing results with other similar studies (“Validation of a simplified AQUATOX model to assess quality status of a model river in Sardinia”).

In particular, these tests’ results underline that anthropological pressures have an higher impact on the biota community and the ecosystem answer compared to the hydraulic behaviour of the stream (and in general to the total water volume of the water body), even in terms of nutrients transportation (and, even more, transformation).

Even if for the “Whole” simulation a decreasing accuracy in time can be noticed, it still remains a good representativeness in terms of LIMeco determination basing on results and so the possibility to involve AQUATOX and this method in long-term river water quality assessment and forecast.

References

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