COMBINED USE OF THE EPA-QUAL2E SIMULATION MODEL AND FACTOR ANALYSIS TO ASSESS THE SOURCE APPORTIONMENT OF POINT AND NON POINT LOADS TO SURFACE WATERS

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ABSTRACT

Diffuse pollution is generally indirectly estimated by area, and specific emission factors as function of land use. However in many cases these estimates were proven to be remarkably wrong. Aim of present study was to combine a water quality simulation model, (USEPA-QUAL2E) and Factor Analysis to increase the understanding of the water pollutants source apportionment. The study concerned two different watersheds, an upland area characterised by a very scarce agricultural use, and another area covering both the upland and the lowland physiographic regions. Particularly the lowland region is included in one of the most productive agricultural areas in Italy. By comparing instream measurements with Qual2E simulations during dry and wet weather conditions, a better fit (errors ± 20%) was found, for the dry weather scenario, revealing the scarcer reliability of the adopted non point emission estimates. Model simulations enabled to estimate the non point contribution to the instream load, that was found around 80% in the area of extensive agricultural land use, and around 40% in the upland region. Moreover Factor Analysis applied to the instream data suggested for the upland region an exchange from the groundwater to the surface water system. This hypothesis was also supported by the QUAL2E simulations.

KEYWORDS: non point pollution, point pollution, QUAL2E, integrated monitoring, nutrients, watershed management

INTRODUCTION

In Italy up to now, diffuse pollution of watersheds has been generally estimated by area-specific emission factors as function of land use (e.g. arable, grasslands, etc.). However, the comparison of instream direct measurements, with the results of a mass balance has suggested in many cases (Zessner and Kroiss, 1999; Svendsen and Kronvang, 1993, Arheimer and Brandt, 1998) that these emission estimates can be remarkably wrong. Assessing the apportionment of point and non point contributions to the instream total load, is also extremely difficult. In fact, although many studies have analysed nutrient emissions from soil to surface water (Burt at *al*., 1992, Tunney et *al.*, 1997 among the others), the spatial and temporal extent of these studies was generally limited. In addition, predicting the point and non point contributions to the stream total load is also hampered by the difficulty of achieving extensive direct measurements of nutrient losses from soil to surface waters at large spatial and temporal scale. Such an evidence makes extremely difficult the validation of any predictive model. Furthermore most software packages, that are commonly used for the river quality modelling (i.e. QUEAL2E, SIMCAT, WASP, SALMON_Q etc.), are intended specifically for the steady-streamflow and the steady-effluent discharge conditions specified in the water quality regulations for wasteload allocations. This is particularly true for the model QUAL2E that is currently considered the standard for the stream quality modelling (Shanahan *et al.*, 1998). As addressed by some authors (Shanahan *et al.*, 1998), in fact, QUAL2E is best suited for point sources of pollutants and has limitations when simulating rivers that experience temporal variations in streamflow in polluting load over a diurnal or a shorter time period. Unfortunately these are severe limitations when considering the non point sources of pollutants which are mostly driven by rainfall events when both the loads and the streamflow vary over time. On this respect it should be also added that currently there is no readily available, widely accepted tool that enables to simulate the river water quality during rainfall events at such large scales (i.e. basin-scale) and over the instantaneous temporal scale which is typical of water quality direct measurements. Nevertheless, on this perspective, a steady-streamflow simulation tool such as QUAL2E has the major advantage of being widespread and readily available, and being intended to simulate at the instantaneous scale, it offers intrinsically the opportunity for validation by the comparing its predictions with direct measurements. Moreover these simulations, when used in combination with other exploratory techniques such as Factor Analysis, shed insights about the relative importance of non point sources to the river water quality. Aim of this study was to combine QUAL2E simulations with the results of a Factor Analysis to study the apportionment of point and non point sources to the river quality of two different watersheds.

DATA AND METHODS

Study Area

Two watersheds were investigated: the Adda upland catchments, characterised by streams with relatively steep slopes and deep-incised channels, encompassed within a largely forested region with some agricultural areas (i.e. vineyards, maize and apple trees) and Cherio basin. Particularly the investigation on Cherio watershed covered two distinct physiographic regions: an upland region similar to the Adda river upland physiography and a lowland region which is encompassed within one of the most productive agricultural region in Northern Italy (i.e. the Po Valley). Table 1 summarises the characteristics of the two study areas, both shown in Fig. 1.

Table 1 - Characteristics of the two study areas.

	Cherio Basin	Adda Basin
Drainage area (km^2)	150	2470
Upland region (%)	68%	100%
Urban areas (%)	26%	0.8%
Agricultural region (%)	32%	5%
Dominant coltures	Maize (59%), Wheat (30%)	Vineyards (2.9%), Maize (50.4%), Apple Trees (8.8%)

Input Data

Measurements of different water quality parameters, coming from the two watersheds, were used to implement the water quality simulations, during dry and wet weather conditions. All the measurements came from to the monthly monitoring activity, carried out by ARPA, the Italian regional environmental protection agency, during the biennial 2000-2001 at 9 sampling stations within the Adda Basin and at the sampling station at the outlet of Cherio river.

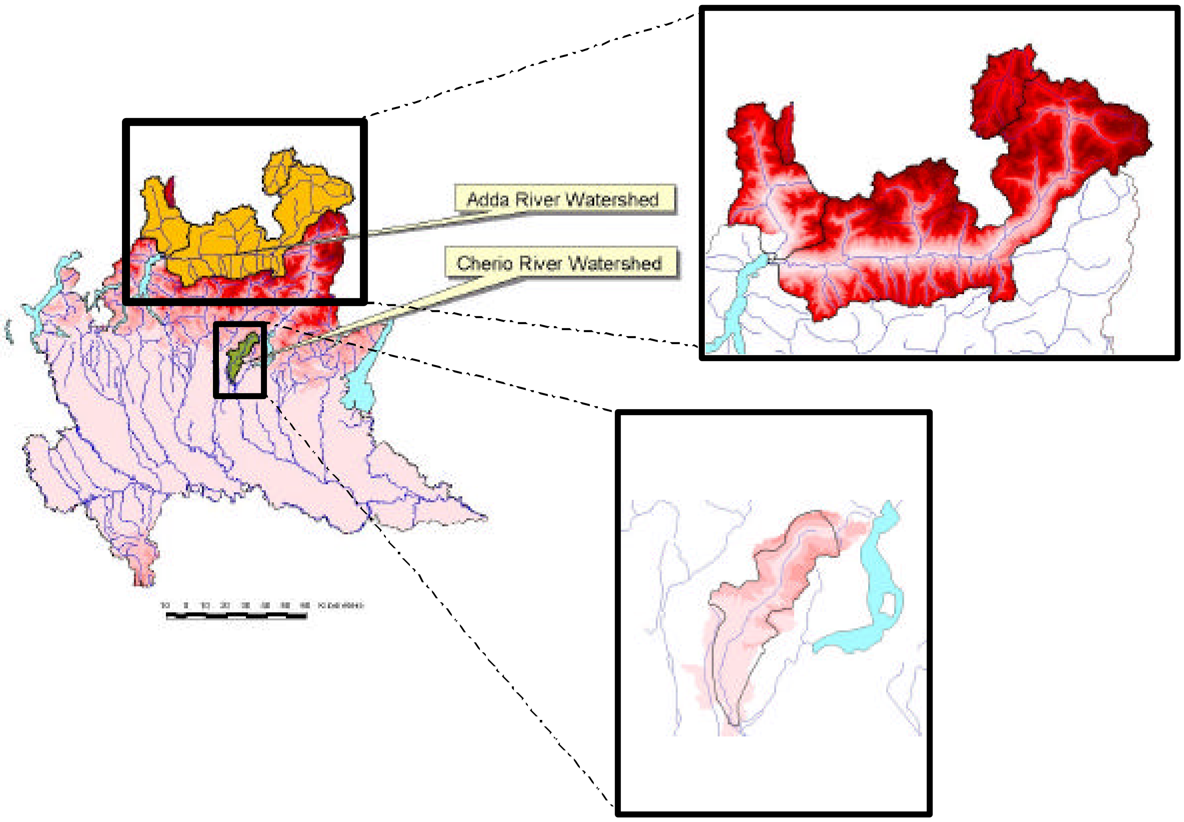


Fig. 1. Study area: Upland Adda River and Cherio River basins. Northern Lombardy, Italy. The Scale bar is 60 km.

QUAL2E Simulations relied on indirect estimations of the input loads, either for point sources, where population equivalent (PE) specific emission factors and average treatment removals were used (Table 2), or for non point sources, for which land use area specific emission factors were used instead (Table 3). Industrial point sources have been estimated on the basis of the industrial typology and the employee number. These emission factors were substantially the same used by the most of the Italian watershed management authorities (e.g. Autorità di Bacino del Po among the others). On the ground of the measurements, nitrogen speciation was assumed as 73% nitrates, 5% ammonia and 22% organic, whereas all the phosphorous was considered dissolved.

Table 2 - Point sources emission factors and average treatment removals used to estimate the domestic wastewater loads.

Pollutant	Emission	Imhoff Removal %	A.S.* Removal %	A.S + N Removal %	F.A. + N, P Removal %
BOD_5	60 g BOD PE^{1} d^{-1}	25	90	92	92
COD	129 g COD PE^{-1} d^{-1}	25	85	85	85
Total-N	12.3 g N PE^{1} d^{-1}	15	35	65	65
Total-P	1.8 g PE^{1} d^{-1}	20	35	35	85

*A.S.: Activated Sludge

Table 3 - Diffuse area specific contributions as function of land use.

Pollutant	Arable	Grasslands	Forest	Other
Nitrogen percolation and runoff kg N/(ha y)	20 – 30	5 – 7	3 –10	5
Phosphorous erosion and runoff kg N/(ha y)	0.5 - 1.3	0.3 – 0.5	0.2 – 0.3	0.2 –0.5

RESULTS AND DISCUSSION

Model Validation

QUAL2E was applied without an ordinary calibration because the necessary input data were not available at the scale of the two basins. Therefore literature values (Bowie *et al.,* 1985) have been used as reference for the constants and rates needed by the model.

Dry Weather scenario

Notwithstanding a sort of model calibration was obtained by feeding the model with the indirect estimates of the input loads, obtained as described in the methods, and by comparing model predictions to the median trend of the measured instream quality of the two rivers. In such a way the median of quality measures collected at every sampling station was compared to the corresponding simulated values. Such a calibration at large (and consequently coarse) spatial and temporal scale was mostly a validation of the rates and constants adopted (Table 4) and corresponded roughly to a mean annual scenario of the impact of point loads on the river quality. As a matter fact the median was preferred to the mean as a more robust estimator of central tendency because of the distribution skewness of the quality measurements.

Table 4 – Rates and constants validated by using the median trend of instream measures.

K_2 ¥	BOD	BOD (s)*	SOD**	N_{org}	N_{org} (s)*	NH_4-N °	NH_4-N°	NO_2-N	P_{org}	P_{org} (s)*	$P_{dissolved}$°	COLI
	d^{-1}	d^{-1}	$g\ m^{-2}\ d^{-1}$	d^{-1}	$g\ m^{-2}\ d^{-1}$	$g\ m^{-2}\ d^{-1}$	d^{-1}	d^{-1}	d^{-1}	d^{-1}	$g\ m^{-2}\ d^{-1}$	d^{-1}
Adda River												
3	0.4	0.08	0	0.16	0.04	0	0.24	0.68	0.01	0.08	0.02	0.03
Cherio River												
3	0.4	0.08	0	0.16	0.04	0	0.39	0.9	0.01	0.09	0.01	0.03

∞ K_2: reareation rate coefficient.
° benthos sources rates for ammonia nitrogen and dissolved phosphorous.
** SOD: Sediment oxygen demand rate
* (σ): Settling rates

Model accuracy over the median annual scenario was quite good for both the studied watershed scenarios. Simulations in both cases showed a reasonable match with measured values (errors ± 20%), as it is presented in Fig.2. These performances were expected since the median annual scenario is a good approximation of the QUAL2E general assumptions (i.e. steady-streamflow and constant emissions).

Wet Weather scenario

The same procedure was attempted for the wet weather scenario (i.e. simulation under rainfall events) even though, as stressed before, rainfall conditions may deviate significantly from QUAL2E assumptions. However in order to avoid the extreme forcing of those assumptions the mean rainfall event was taken as reference. In such an average scenario the land use, area-specific emission factors allowed to estimate the mean contribution of diffuse load during rainfall events. In such a way non point input loads were calculated on the basis of the annual statistics obtained from the emission factors and were distributed over the monthly average of rainy days and of cumulative precipitations (mm). Then to obtain pseudo-instantaneous loads the estimated diffuse emissions were converted in kg s^{-1} (Fig. 3). In contrast with what came out from the dry-weather scenario, the wet-weather simulation outlined a remarkable overestimation of the instream load (in some occasions errors were much higher than 100% and up to a 3-4 timesfold overestimation).

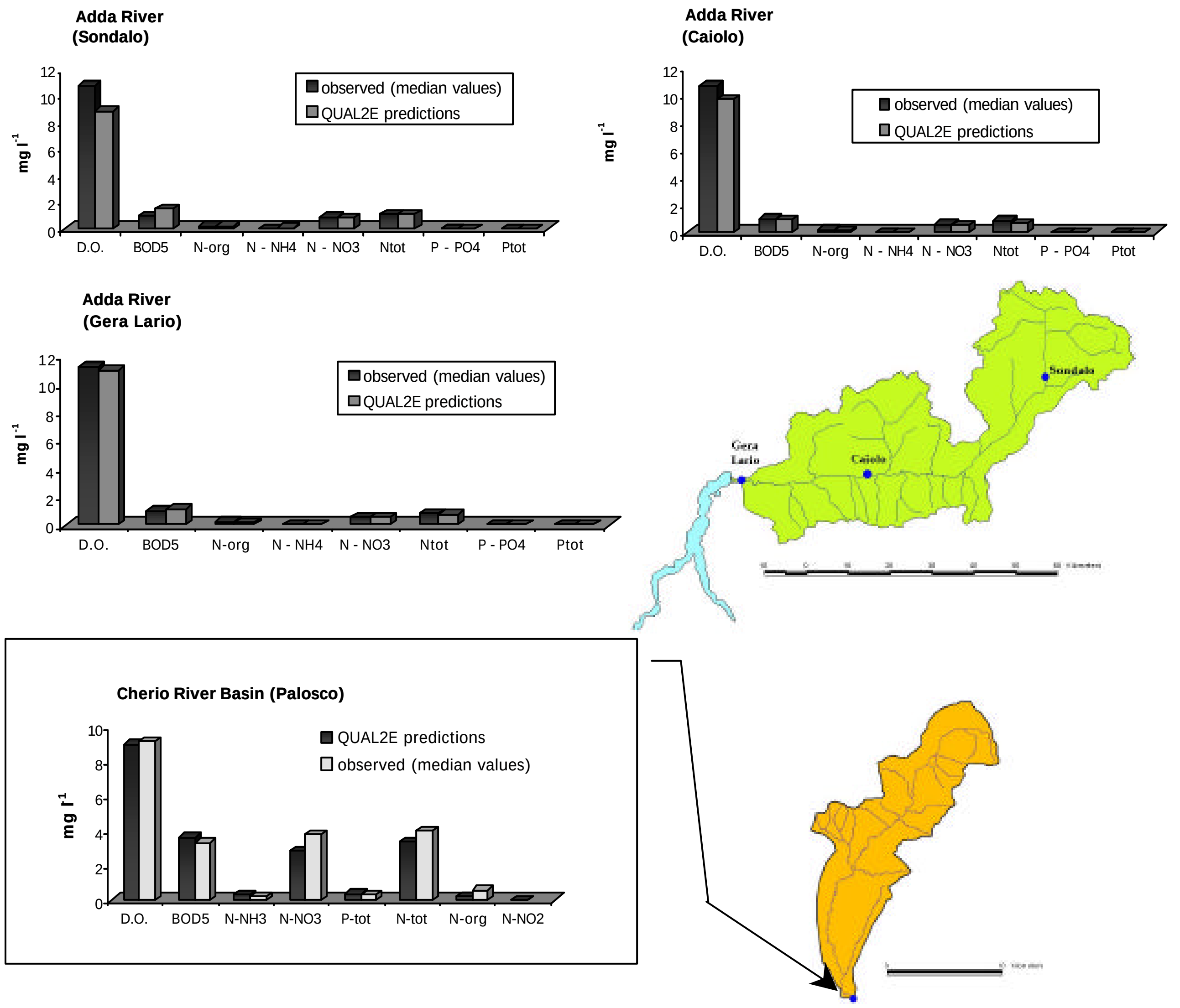


Fig.2. Validation of QUAL2E model for the two study cases. In both cases the match between predictions and observed values was quite good (dry weather conditions).

This overestimation was the effect of the non point loads and revealed the coarseness of non point with respect to point source emission estimates. Besides these findings agree with what was found within the study “Nutrient Balances for Danube Countries” (Danube Applied Research Program, Project EU/AR 102A/91, 1997) that outlined a significant overestimation (about 3-3.5 timesfold) of the nitrogen and phosphorous emissions, estimated with indirect load-emission coefficients similar to the ones used here, to the surface waters in Danube Basin. Moreover, by simulating the same scenario considering only point sources (where volumes discharged were increased by 25%, obtaining consequently more diluted point loads) and then subtracting the point sources contribution from the instream total load obtained by measurements, non point sources’ contribution, was found around 80% of the instream total load in an area of extensive agricultural land use as Cherio Basin (Fig.4b), and around 40% in the Upland Adda watershed (Fig.4a).

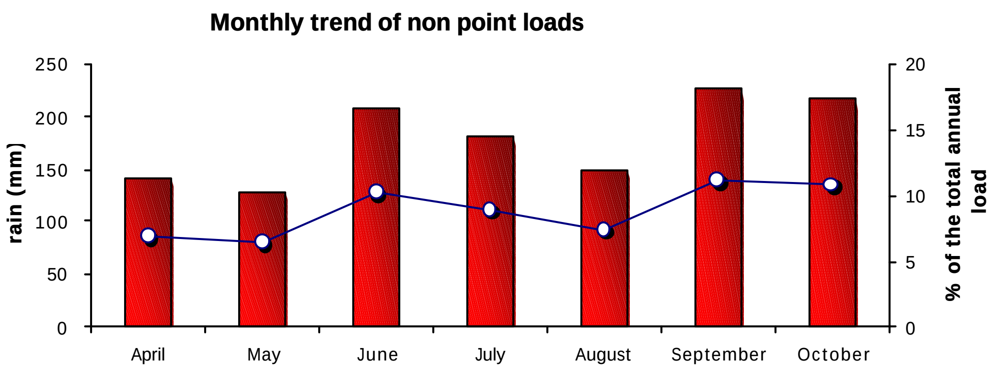
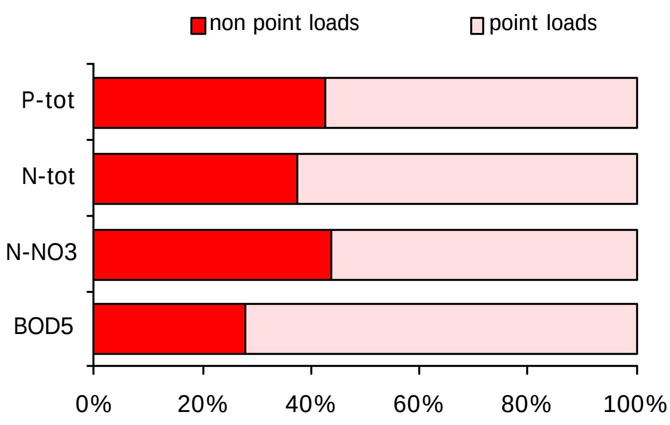


Fig. 3. Theoretical monthly trend of non point loads assumed for QUAL2E simulations. The annual non point contribution to the instream load was distributed on a monthly basis following the cumulative precipitations trend (bars). Dots represent the monthly percentage of the annual total diffuse load to surface waters.



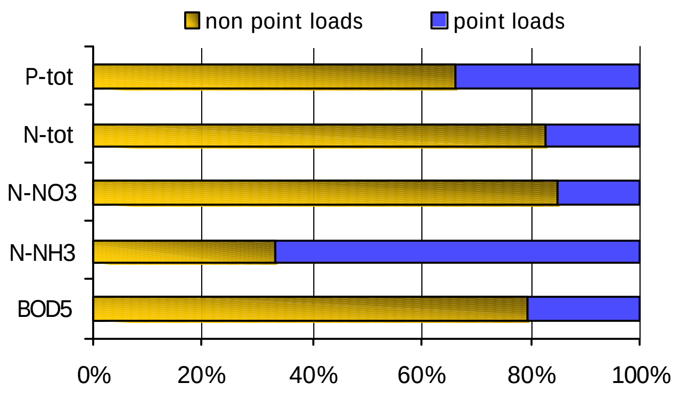


Fig.4. Point and non point load apportionment obtained by substracting from the measured instream total load the point sources contribution obtained by QUAL2E simulations: (left) Adda River and (right) Cherio River Watersheds.

Factor Analysis

A Factor Analysis applied with a VARIMAX rotation to the water quality measurements of the two studied watersheds, gave further insights on the source apportionment of water pollutants and evidenced finer differences between Cherio and Adda basins. Since based on the measurements which are mostly done during dry weather conditions, Factor analysis reflected also the dry weather scenario where the point sources are the only direct contribution to the stream total load. Notwithstanding interesting findings have came out.

<u>Adda River Basin (Upland)</u>

Six factors were extracted on the basis of their eigenvalue higher than 1 for a total explained variance of 73.3% (see Table 5). As showed by the factor loadings matrix, nitrates and nitrites surprisingly were loaded on different factors, being nitrates associated to chlorides on factor 2 (explained variance: 16.6 %) and nitrites loaded with dissolved oxygen and *E.coli* on factor 4 (explained variance: 8.8 %).

Table 5 – Adda River Basin: factor loadings matrix.

Factor Loadings (VARIMAX Rotation)						
	Factors					
	1	2	3	4	5	6
PH	0.526	0.017	-0.023	0.415	0.099	-0.426
Conductivity	0.920	0.160	0.013	-0.017	-0.014	-0.047
Hardness	0.961	0.151	-0.013	0.015	-0.013	-0.079
Suspended material	0.017	-0.167	-0.065	0.080	0.717	-0.199
Dissolved Oxygen	0.061	0.016	0.151	0.567	-0.363	-0.112
Total Nitrogen	0.161	0.916	0.141	-0.001	0.008	0.005
N-NO3	-0.062	0.944	0.026	0.005	0.021	-0.008
P-PO4	0.042	0.022	0.879	0.123	0.092	0.050
Total Phosphorous	-0.025	0.087	0.863	0.070	-0.093	-0.134
Chlorides	0.199	0.798	-0.025	0.123	-0.063	-0.104
Sulfates	0.954	-0.013	0.027	-0.101	-0.046	0.061
E.coli	-0.114	0.160	0.184	0.623	0.298	-0.135
Extended Biotic Index (IBE)	-0.040	-0.067	-0.067	-0.074	-0.038	0.818
Zn	-0.023	0.101	0.065	-0.012	0.696	0.114
N-NO2	-0.045	-0.035	-0.038	0.622	0.076	0.525
% Explained Variance	20.3	16.6	10.7	8.8	8.4	8.3
% Cumulative explained variance	20.3	37.0	47.7	56.5	64.9	73.3

This evidence is also reflected by the significant correlation (r: 0.724; p-level < 0.001 n: 180) found between nitrates and chlorides and the lack of such correlation between nitrates and nitrites (r: -0.153; p-level > 0.25 n: 55). Such a pattern suggests for nitrates a different apportionment than nitrites. Nitrites, in fact, being loaded on factor 4, together with dissolved oxygen and *Escherichia coli*, can be associated with urban point source emissions, whereas the relationship found between nitrates and chlorides, suggests an exchange from the groundwater to the surface water system ($N\text{-}NO_3$ and Cl^- concentrations in groundwater are much higher than in surface waters). This hypothesis is also supported by QUAL2E simulations, which came up with a systematic underestimation of nitrates reaching a maximum of -11% at Caiolo site.

Cherio River Basin (Lowland)
Five factors were extracted on the basis of their eigenvalue higher than 1 for a total explained variance of 84.1% (see Table 6). In this case no relationship was found between nitrates and chlorides and nitrates were loaded on factor 4 together with pH, hardness and conductivity. Moreover the first two factors that loaded respectively *E.coli*, dissolved phosphorous, ammonia and total nitrogen, the first, and the organic matter and total phosphorous, the second, explained almost 50% of the variance revealing a completely different scenario from the upland, with pollutants far more linked to the suspended rather than to the dissolved fraction.

CONCLUSIONS

Despite the fact that QUAL2E is a model built under severe assumptions that strongly limit its applicability to non steady state scenarios, still it offers the opportunity for a validation at a coarse scale of the non point emissions estimates that are commonly employed by watershed authorities to manage nutrients reduction at the watershed scale. By comparing model predictions with direct measurements it was possible to quantify the huge overestimation introduced by these emission coefficients. Moreover these simulations, when used in combination with Factor Analysis, may show hidden features such as the groundwater exchanges to the surface water system, giving insights about the effect of non point sources on the instream water quality also during dry weather conditions.

Table 6 – Cherio River Basin: factor loadings matrix.

Factor Loadings (Varimax Rotation)					
	Factors				
	1	2	3	4	5
Dissolved Oxygen	-0.097	-0.361	0.669	-0.009	-0.276
BOD5	0.595	0.779	-0.004	0.027	0.046
COD	0.347	0.888	-0.034	0.074	-0.002
E. coli	0.873	0.363	0.085	0.090	-0.102
N-NH4	0.957	0.107	0.039	0.067	-0.076
N-NO3	0.000	0.082	0.146	0.852	0.196
Total Phosphorous	0.663	0.641	0.126	0.200	0.190
P-PO4	0.827	0.211	0.355	0.110	0.156
Total Nitrogen	0.860	0.036	0.137	0.419	0.127
PH	-0.301	-0.019	0.356	-0.677	0.013
Conductivity	0.293	-0.296	0.341	0.675	-0.286
Hardness	0.140	-0.618	-0.005	0.544	-0.290
Suspended solids	0.082	0.884	0.090	-0.149	-0.236
Chlorides	0.438	0.125	0.746	0.119	0.273
Sulfates	0.262	0.186	0.791	0.018	0.012
Extended Biotic Index (IBE)	0.123	-0.134	-0.041	0.004	0.858
Temperature	-0.461	0.375	0.433	0.072	0.511
% Explained Variance	27.8	21.1	13.3	13.1	8.8
% Cumulative Explained Variance	27.8	48.9	62.2	75.3	84.1

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