18th World IMACS / MODSIM Congress, Cairns, Australia 13-17 July 2009
http://mssanz.org.au/modsim09

Parameter uncertainty analysis of water quality model for small river

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Abstract: Every model is, by definition, a simplification of the reality under investigation. Although it would be desirable to reduce to zero the gap between the simulated and the observed system behavior, this is generally impossible owing to the unavoidable uncertainties inherent in any modeling procedure. In literature, generally, these prediction uncertainties are linked to measurement errors associated with system input and output, to the incapacity of calibration procedures and, finally, to the model structural errors arising from the aggregation of real world process into a modeling simplification.

In this context, a good modeling practice requires that the modeler provides an evaluation of the confidence in the model, possibly assessing the uncertainties associated with the modeling process and with the outcome of the model itself.

A measure about the significance of the model results in order to understand the level of confidence characterize them is necessary. With this regards, uncertainty analysis can provide useful hints as well as information regarding the best model approach to be used with respect to its significance and reliability degree. Further, the evaluation of parameter uncertainties is necessary to estimate their impact on model performance and for their calibration (Beck, 1987).

More specifically, uncertainty and sensitivity analysis can offer valid tools for characterizing the uncertainty associated with a model. In any case, sensitivity analysis may help understanding the contribution of the various sources of uncertainty to the model output uncertainty and system performance in general. Then, uncertainty is a measure of the 'goodness' of a result; without such a measure, it is difficult to judge the fitness of the value as a basis for making decisions relating scientific excellence.

In this context the uncertainty of a river water quality model is presented. The main goal is to gain insight in the modeling approaches concerning small rivers. Indeed, previous works generally focused on modeling of large river neglecting the small one. Such aspect is likely due to the fact that small river are often considered unworthy from practical and economic viewpoint (Marsili-Libelli and Giusti, 2008). However, such considerations are not completely fulfilled for Mediterranean region where there is a strong variably among the seasons and therefore the rivers are generally ephemeral (i.e. river characterized by long dry season and intense flow for short periods following precipitations). This aspect is relevant since the role played by the physical/chemical/biological processes is different and the parameter values are different of order of magnitude. In order to demonstrate such fact, a simplified river water quality model was calibrated after an extensive data gathering campaign on an Italian river. Following a model calibration, the model uncertainty has been assessed by means of the GLUE (Generalized Likelyhood Uncertainty Estimation). The results showed that small rivers have different behaviors respect to the large ones in terms of importance of physical chemical processes. Such fact is reflected on the parameter values of the kinetic constant that are order of magnitude different from the large river ones. On the other hand, concerning the model uncertainty assessment, the uncertainty bounds were found to be relatively wide. These results have revealed that the model is unable to reproduce the pollutant discharges consistently and that the resulting predicted pollutant loads must be associated with significant uncertainty. This may be due in part to interaction between model parameters leading to equifinality between parameter sets. However, in terms of model capability to reproduce measured data, the results are in good agreement with the observed water quality data, therefore the model is consistent and can be a useful tool for water resource management.

Keywords: *integrated urban drainage modeling, uncertainty assessment, model approaches, water quality management*

1. INTRODUCTION

In the last decades, public awareness about environment is improving and the impact of wastewater discharges on the dissolved oxygen of water bodies is receiving even more attention.

The importance of receiving water body quality state is also presented in the EU Water Framework Directive 60/2000 that proposes a water-quality oriented view of the whole system and entails new sustainable approaches for disposing of stormwater (Chave, 2001).

Water quality models are often implemented in order to quantify the substance transformation and to investigate the impact that changed boundary conditions have on the aquatic system (Wagenschein and Rode, 2008). However, especially for small river, some problems hamper a straightforward model application basically due to data scarcity, lack of major investments as a consequence of their minor importance, and the large number of diverse inputs, especially if they flow through densely populated areas (Marsili-Libelli and Giusti, 2008). These facts constitute the major complicatedness in the application of water quality models, such as those provided by the US Environmental Protection Agency: QUAL2E (Brownand Barnwell, 1987), QUAL2K (Chapra and Pellettier, 2003), WASP6 (Wool et al., 2006), or the IWA River Quality Model No. 1 (Reichert et al., 2001), which require more information regarding the river system than is often available. For these reasons Marsili-Libelli and Giusti (2008) suggest to employ *ad hoc* simple models in order to derive the crucial information about the river quality and become part of a decision support system. Moreover there is a need of a measure about the significance of the model results in order to understand the level of confidence characterize them is necessary. With this regards, uncertainty analysis can provide useful hints as well as information regarding the best model approach to be used with respect to its significance and reliability degree. Further, the evaluation of parameter uncertainties is necessary to estimate their impact on model performance and for their calibration (Beck, 1987).

The origin of uncertainty should be identified before studying its effect on simulation results (Dubus et al., 2003). Previous research on the uncertainty analysis in environmental models generally addressed three types of uncertainties: structure uncertainty, input data uncertainty and uncertainty of the model parameters values (Harremoës, 1988; Refsgaard et al., 2007; Freni et al., 2009). Structural uncertainty is due to the lack of complete understanding of physical, chemical, and biological processes and the conceptual simplification of these processes using mathematical functions. It may result from: (1) the assumptions and simplification in the model and (2) application of the model under conditions that are not quite consistent with the model design (Tripp and Niemann, 2008). In general, researchers study the structural uncertainty by comparing different models, and improving the models is the main way to overcome this aspect of uncertainty. The uncertainty of model input occurs because of changes in natural conditions, limitations of measurement, and lack of data (Beck, 1987). One way to deal with this issue is to use random variables as the input data, rather than the conventional form of fixed values. The uncertainty of model parameters arises because parameters attained through empirical estimation and optimization of observed data cannot ensure the precision and reliability of the predicted results (Beck, 1987).

When dealing with complex modeling approaches in a context with limited data, classical calibration approaches may lead to several equally consistent parameters sets and it is difficult to have sufficient confidence about the obtained results (Sorooshian and Gupta, 1983).

These considerations lead to the equifinality concept accepting the fact that more parameter sets may exist able to provide a good fit between simulated and measured data. During the last years, several approaches have been developed on the basis of accepting non-uniqueness of calibrated parameters. The non-uniqueness of parameter calibration set and the uncertainty connected to their estimation take the primary consequence that, for a given model structure and a given experimental layout, some modeling parameters cannot be reliably calibrated because the available information is not adequate to identify their specific effect on modeling output. One such method is the Generalized Likelihood Uncertainty Estimation (GLUE) developed by Beven and Binley (1992). The GLUE has been extensively used for simultaneous calibration and uncertainty assessment especially for hydrologic models (Lamb et al., 1998; Freer et al., 2004). The GLUE, compared to other methods, is easy to implement and allows a flexible definition of the so-called likelihood function used to separate behavioral and non behavioral solutions. The likelihood function can include several variables, a feature that is particularly valuable for assessment of integrated, distributed models that operate with multi-variable, multi-site and multi-response criteria. The main drawbacks of the GLUE technique are the subjectivity involved in the definition of the likelihood function and the threshold for defining the behavioral solutions and the huge number of necessary model simulations (Freni et al., 2008).

In this frame, the paper presents the uncertainty assessment of a water quality model for small rivers by means of the GLUE. The model has been applied to the Oreto river which is located in Sicily (Italy). The river has been an object of an Italian research project aimed to the assessment of its quality status and, for this reason, several monitoring campaigns have been carried out in order to collect quantity-quality data.

2. THE MODEL

A modified version of the Streeter-Phelps model has been considered for the evaluation of the receiving water body quality state. More specifically, in the case of one dimensional flow, the advection-dispersion equation can be formulated as in the following (Thomann and Mueller, 1987; Chapra, 1997):

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}=D_L\frac{\partial^2 C}{\partial t^2}-f(C) \qquad (1)$$

where C is the concentration of a generic pollutant, t is the time, x is the longitudinal displacement, u is the velocity of and D_L is the diffusion coefficient, f(C) is the generic reactive term for the pollutant C. Neglecting the diffusion term, and after mathematical manipulation Eq. (1) becomes:

$$\frac{dC}{dt}=\frac{\partial C}{\partial x}\frac{dx}{dt}+\frac{\partial C}{\partial t}=\frac{\partial C}{\partial x}u+\frac{\partial C}{\partial t}=-f(C) \qquad (2)$$

Concerning the reactive processes the following terms have been considered:

- degradation of dissolved carbonaceous substances;
- ammonium oxidation;
- algal uptake and denitrification;
- dissolved oxygen balance, including depletion by degradation processes and supply by physical reaeration and photosynthetic production.

In figure 1 the interconnections about the modeled process are reported along with the main model variables considered. Dissolved oxygen is produced by reaeration through interchange with the atmosphere and photosynthesis of algae and plants. On the other hand, the oxygen is consumed by respiration of microorganisms, aquatic plants, and bacteria. These bacteria act as catalyser for the degradation of organic material (BOD decay), by which oxygen is consumed. Other processes which consume oxygen are the oxidation of nitrogen compounds (e.g. nitrification or the oxidation of NH_4 to NO_3) and the sediment oxygen demand. This oxgygen demand originates from the degradation of deposited organic matter. In addition, oxygen is reaerated through interchange with the atmosphere. Similarly to Marsili-Libelli and Giusti (2008) model approach, phosphorus was not included in the model because for the selected case study, discussed in the following, in the river its concentration was too low to be observed and modelled reliably. Further, almost the entire algal population is composed by N-limited species and its interaction with dissolved inorganic nitrogen is described by the preferential absorption coefficient δ introduced by Brown and Barnwell (1987) in the QUAL2 model family. Concerning the simulated model variables the following equations have been employed:

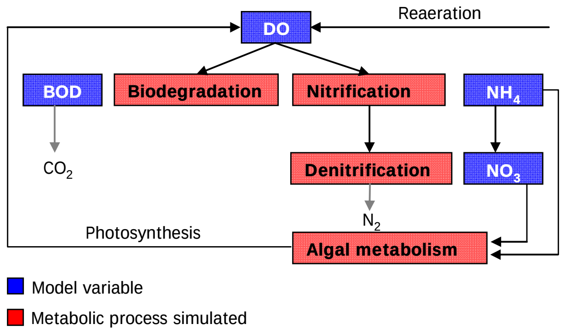

Figure 1. Modeled transformation processes.

$$\frac{dBOD}{dx}=-\frac{1}{u(x)}\cdot k_D\cdot BOD \qquad (3)$$

$$\frac{dNH_4}{dx}=-\frac{1}{u(x)}\cdot k_N\cdot NH_4-\frac{1}{u(x)}\cdot\delta\cdot k_{Al}\frac{NH_4}{k_f+NH_4} \qquad (4)$$

$$\frac{dNO_3}{dx}=-\frac{1}{u(x)}\cdot k_{Den}\cdot NO_3+\frac{1}{u(x)}\cdot k_N\cdot NH_4-\frac{1}{u(x)}\cdot(1-\delta)\cdot k_{Al}\frac{NO_3}{k_f+NO_3} \qquad (5)$$

$$\frac{dO_2}{dx}=\frac{1}{u(x)}\cdot k_R\cdot(O_{2SAT}-O_2)-\frac{1}{u(x)}\cdot k_D\cdot BOD-Y\cdot\frac{1}{u(x)}\cdot k_N\cdot NH_4+Ph \qquad (6)$$

where k_D is the deoxygenation coefficient, k_N is the nitrogen coefficient, k_{Den} is the denitrification coefficient, δ the preferential absorption coefficient, k_{Al} is the nitrogen algal uptake coefficient, k_R is the reareation constant, Y is the autotrophic organism yield factor, Ph is the actual production of oxygen due to photosynthesis and O_{2SAT} is the oxygen saturation concentration.

3. UNCERTAINTY ANALYSIS BASED ON THE GLUE METHODOLOGY

The GLUE methodology was first proposed by Beven and Binley (1992) as a framework for the estimation of uncertainty from equally acceptable models or parameter sets. In the present study, it will be used for assessing the parameter uncertainty in small river modelling. By means of a likelihood measure parameter sets are classified and sets with poor likelihood weights, with respect to a user-defined acceptability threshold (Tr), are discarded as “non-behavioural”. All parameters sets coming from the behavioural simulation runs are retained and their likelihood weights are re-scaled so that their cumulative total sum is equal to 1. The likelihood measure represents the ability of the model to fit real data. On the other hand, the acceptability threshold, Tr, represents a user-defined critical value indicating the minimum value of the likelihood measure that each modelling simulation should have to be representative of the model behaviour with respect to the analysis aim. Tr is usually set equal to zero. In the present study, the Nash and Sutcliffe efficiency index has been used as likelihood measure (Nash and Sutcliffe, 1970):

$$L(\theta_i/Y) = \left(1 - \sigma_i^2/\sigma_0^2\right) \qquad \sigma_i^2 < \sigma_0^2 \tag{7}$$

where L(θ_i/Y) is the likelihood measure for the ith model simulation for parameter vector θ_i conditioned on a set of observations Y, σ_i^2 is the associated error variance for the ith model and σ_0^2 is the observed variance for the period under consideration. Like other likelihood measures, Nash - Sutcliffe index is equal or lower than zero for all simulations that are considered to exhibit behaviour dissimilar to the system under study, and it increases monotonically as the similarity in behaviour increases with a limit value equal to 1. Once defined a likelihood index, the likelihood value associated with a set of parameter values may be treated as a fuzzy measure that reflects the degree of belief of the modeller in that set of parameter values as a simulator of the system. The degree of belief is derived from the predicted variables arising from that set of parameter values. Treating the distribution of likelihood values as a probabilistic weighting function for the predicted variables, therefore allows an assessment of the uncertainty associated with the predictions, conditioned on the definition of the likelihood function, input data and model structure used.

A method of deriving predictive uncertainty bounds using the likelihood weights from the behavioural simulations has been shown by Beven and Binley (1992). The uncertainty bounds are calculated using the 5% and 95% percentiles of the predicted output likelihood weighted distribution. The bounds width is an indirect measure of the uncertainty connected with modelling approach and the presence of measures outside the uncertainty bounds is a symptom the modelling hypotheses should be rejected. In the specific study, uncertainty connected with both quantitative and qualitative objective functions has been analysed and they will be described in the following paragraphs. For running the GLUE analysis, a uniform distribution has been considered (Beven and Binley, 1992). The uncertainty assessment has been based on 10,000 behavioural Monte Carlo simulations.

4. THE CASE STUDY

The model and the uncertainty analysis have been applied to the Oreto river (Italy). The catchment of the Oreto river is located near Palermo in the north-western part of Sicily, Italy (Figure 2) and is characterized by an area of 110 km^2. Residential, commercial, farm and industrial settlements cover almost the entire area. The catchment can be considered as geologically homogenous, the dominant rock types are limestone, clay, siltstone and dolomite, the pervious area is about 67%. Vegetation is characterized by weeds, tree-shrub formations, known locally as Mediterranean bush and some agricultural plots; the higher elevations are covered by pinewood forests and, occasionally, cork oaks. The climate is Mediterranean with hot dry summer and rainy winter season from October to April. The hydrological response of this basin is dominated by long dry seasons and following wetting-up periods, during which even large inputs of rainfall may produce little or no response at the basin outlet. The catchment receives yearly approximately 1030 mm of precipitation, producing a mean annual runoff of 450 mm at the mouth. The measurement network consists of six raingauges, spread over the catchment and managed by the Regional Hydrographic Service, and of one level gauge, (named “Oreto a Parco”), located 10 km upstream the river mouth with a catchment area of 77 km^2. The river receives a number of point discharges from small villages and some outskirts of Palermo, most of them untreated. The river has been monitored in 12 cross sections (Figure 2).

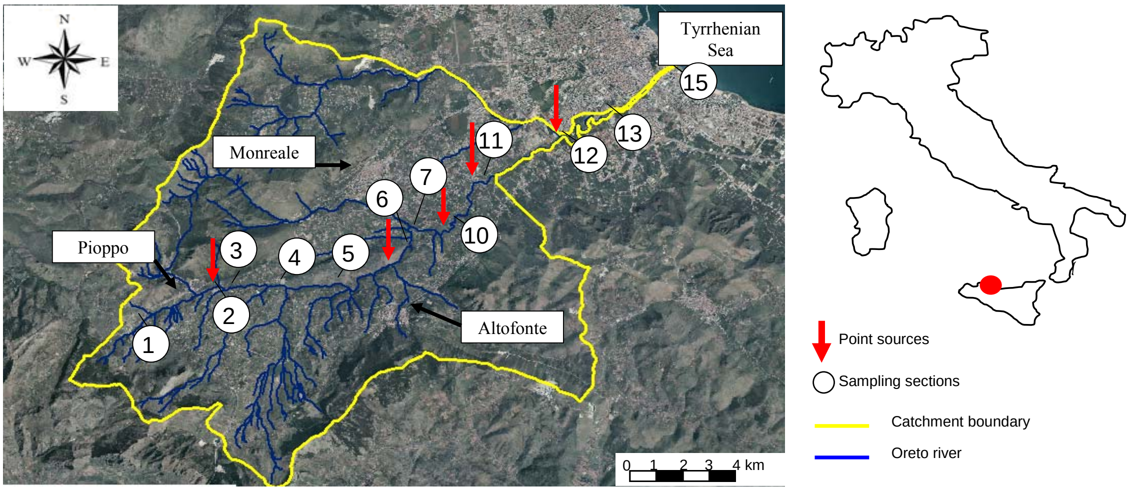

Figure 2. Oreto catchment and sampling sections considered in the monitoring campaign.

For each cross section both quantity and quality data has been collected. In particular, concerning the quality data the following parameters were assessed: water temperature, dissolved oxygen (DO), biochemical oxygen demand (BOD), chemical oxygen demand (COD), ammonia nitrogen, nitrite plus nitrate nitrogen, suspended solids, total phosphorus and ortho-phosphate, in order to describe physical, chemical and microbiological characteristics of the river water. Stream water samples were collected approximately once every three months from January 1998 to December 1999. Therefore, a total of seven measuring campaigns have been carried out building a discrete data base for the assessment of the river quality state. Concerning the morphological aspects, two main stretches have been identified for the Oreto (Figure 3). The river is more pronounced in the upstream part (average slope equal to 4.6%), up to Altofonte, and decreases in the final part (average slope equal to 1.1%). However due to the fact that the major tributaries are located in the upstream part, the final part of the river is much richer in flow and speed than the upstream part and therefore it is more fast-flowing than the upstream one. Due to such division into two different stretches, the model parameters, as will be better discussed in the following, have been calibrated accordingly for each stretch.

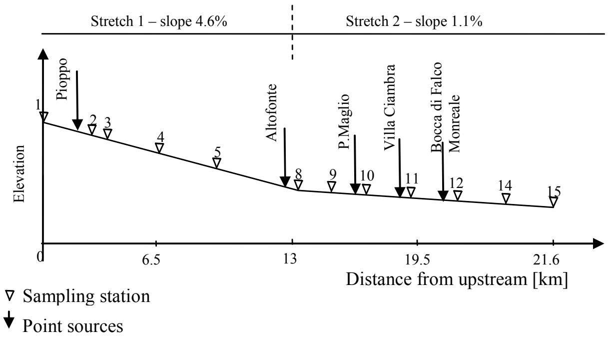

Figure 3. Oreto river schematization.

5. RESULTS

Model application has been carried out following a step wise procedure. More specifically, first the model parameters have been determined and thereafter the model uncertainty expressed in terms of uncertainty bands have been assessed. A Monte Carlo procedure was used to generate large numbers (10^4) of sets of parameters for the model, each parameter value being drawn from ranges thought feasible for the Oreto catchment on the basis of physical argument and previous experience. Simulations were performed for each parameter set for comparison with the measured data (BOD, O_2, NH_4 and NO_3).

The evaluation of the parameter values have been carried out employing the equation (7) where the model state variables (BOD, O_2, NO_3 and NH_4) have been changed in relation to the model parameters to be seek. More specifically, first the deoxigenation coefficient (k_D) has been assessed considering as model state variable the BOD. Thereafter, the evaluation of k_{AL} and k_D coefficients (eq. 4) have been carried out selecting as state variable NH_4. Once evaluated k_D, k_{AL} and k_D their values have been kept constant and k_R and Ph have been assessed by means of eq. 6 selecting as state variable O_2. Finally, the value of the parameter k_{DEN} has been assessed maintaining the other model parameter values constant and selecting NO_3 as model state variable. For each of the four steps discussed above, 10000 uniform random sets of parameters have been generated and these sets have been used to perform model simulation. For each of these simulations a performance index has been evaluated in the form of Nash and Sutcliffe (eq. 7).

Figure 4 shows scatter plots for the likelihood based on (7) for each of the parameters sampled for the model. Each dot represents one run of the model with different randomly chosen parameter values within the selected ranges. The generation of the likelihood surface involves a decision about the criterion for model rejection; actually the uncertainty bounds associated with the retained simulations will depend on the choice of the likelihood measure and rejection criterion. Indeed, as discussed in the previous paragraph, simulations that achieve a likelihood value less than zero are rejected as non-behavioral. The remaining are rescaled between 0 to 1 in order to calculate the cumulative distribution of the predictive variables.

These plots show a strong sensitivity of some model parameters, such as k_D, k_N, and an insensitivity of others such in the case of Ph. Simulations that achieve a likelihood value of zero are rejected as non-behavioral. Following the rejection of non-behavioral simulations, the weights rescaled between 0 and 1 have been applied to their respective model pollutant discharges to give a cumulative distribution of pollutant discharges at each time step, from which the chosen discharge quantiles, 5 and 95%, have been calculated to represent the model uncertainty.

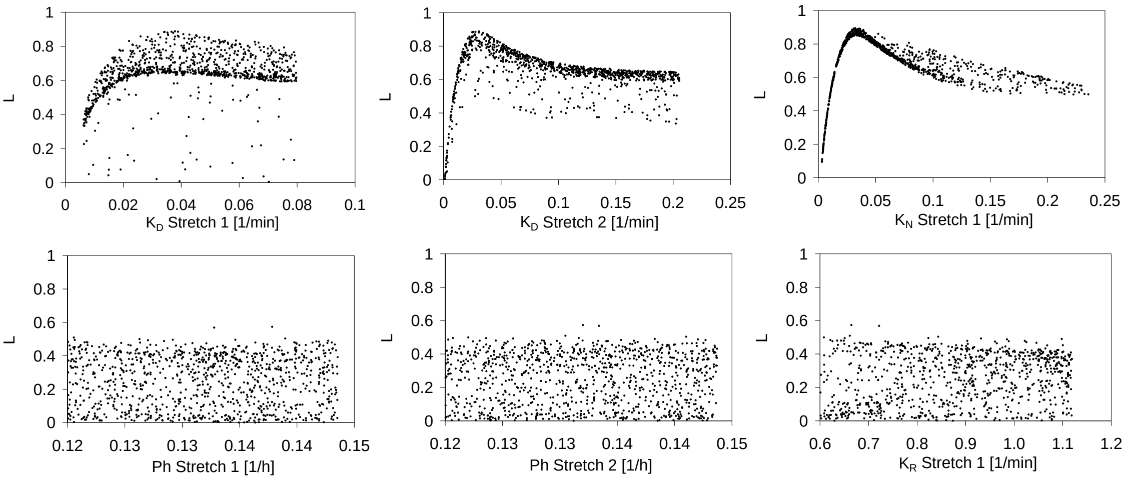

Figure 4. Scatter plots illustrating the distribution of likelihood weighted qualitative parameter values.

Figure 5 shows the pollutant discharge prediction bounds calculated for the BOD, O_2, NH_4 and NO_3, based on the likelihood measure of equation (7). Predicted observable pairs corresponding to the 5% and 95% percentiles limits of the cumulative distributions are used to estimate uncertainties in the model predictions. For the selected pollutant species uncertainty bounds were found to be relatively wide and embrace the measured values.

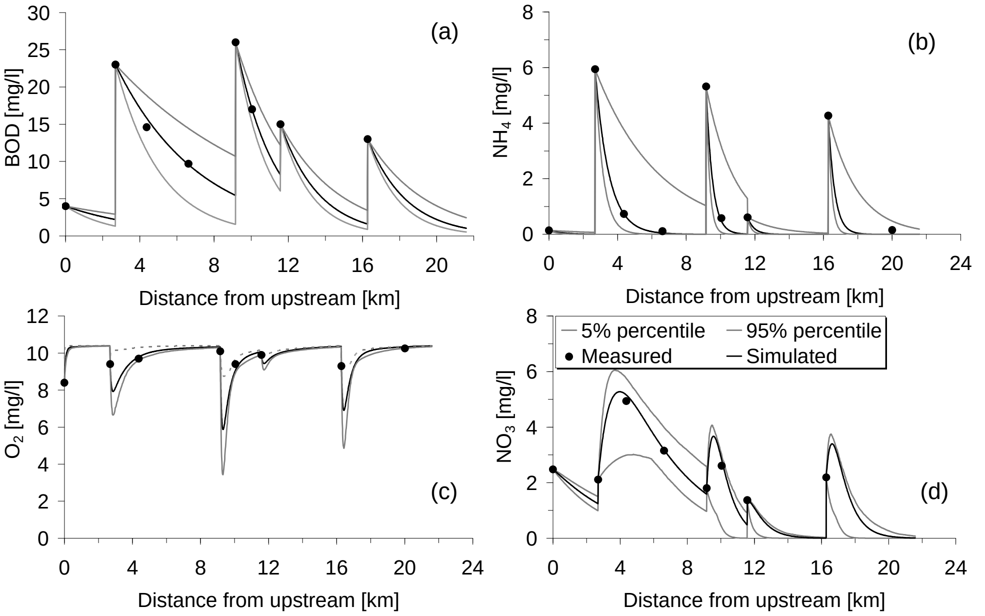

Figure 5. Model results in terms of (a) BOD, (b) NH_4 ,(c) O_2 and (d) NO_3 for the July 1999 campaign.

6. CONCLUSIONS

This paper presented the results of applying the GLUE methodology to a quality model aimed to assess the ecological status of small rivers. The modeling strategy was directed to a simple model because it provides good predictive accuracy in low-yielding rivers, especially when only few and irregularly sampled data are available. The effectiveness of this approach has been carried out with reference to the interpretation of quality field data. The GLUE approach focuses on the issues of the quantitative model prediction, uncertainty and sensitivity inherent in the predictions of pollutant characteristics. GLUE provides an estimate of the likelihood of a model given the observations and thereby includes the effects of model structural error implicitly. The resulting prediction limits were, however, quantiles of the model predictions, not direct estimates of the probability of simulating a particular observation, which is not easily estimated given model structural error. For the analyzed pollutant species uncertainty bounds were found to be relatively wide. These results revealed that the model were unable to reproduce the pollutant discharges consistently and that the resulting predicted pollutant loads must be associated with significant uncertainty. This may be due in part to interaction between model parameters leading to equifinality between parameter sets. In terms of model capability to reproduce measured data, the results were in good agreement with the observed water quality data, therefore the model is consistent and can be a useful tool for water resource management.

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