

Uncertainty estimation of a complex water quality model: GLUE vs Bayesian approach applied with Box – Cox transformation

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Abstract: In urban drainage modelling, uncertainty analysis is of undoubted necessity; however, several methodological aspects need to be clarified and deserve to be investigated in the future, especially in water quality modelling. The use of the Bayesian approach to uncertainty analysis has been stimulated by its rigorous theoretical framework and by the possibility of evaluating the impact of new knowledge on the modelling estimates. Nevertheless, the Bayesian approach relies on some restrictive hypotheses that are not present in less formal methods like GLUE. One crucial point in the application of Bayesian methods is the formulation of a likelihood function that is conditioned by the hypotheses made regarding model residuals. Statistical transformations, such as by the use of the Box–Cox equation, are generally used to ensure the homoscedasticity of residuals but this practice may affect the reliability of the analysis leading to a wrong estimation of the uncertainty. The present paper aims to study the impact of such a transformation considering five cases one of which is the “real” residuals distributions (drawn from available data). The analysis was applied to the Nocella experimental catchment (Italy) which is an agricultural and semi-urbanised basin where two sewer systems, two wastewater treatment plants and a river reach were monitored during both dry and wet weather periods. The results show that the uncertainty estimation is greatly affected by residual transformation and a wrong assumption may also affect the evaluation of model uncertainty. The use of less formal methods always provide an overestimation of modelling uncertainty with respect to Bayesian method but such effect is reduced if a wrong assumption is made regarding the residuals distribution. If residuals are not normally distributed, the uncertainty is over-estimated if Box-Cox transformation is not applied or non calibrated parameter is used.

Keywords: Bayesian inference, Environmental modelling, GLUE, Integrated urban drainage systems, Receiving water body, Wastewater treatment plant.

1. INTRODUCTION

Up to day, although several models have been developed, integrated urban drainage modelling still presents numerous difficulties. The field data needed for model calibration/validation are generally limited and monitoring campaigns are usually characterized by measurements carried out at the watershed outlet, thus being representative of the combined effects of both the accumulation and transport of pollutants throughout the overall system (Ashley et al., 2004; Kanso et al., 2006). The unbalance between data availability and model complexity reduces the reliability of model results, transferring uncertainty to the model outputs. Data and parameters uncertainties are often lumped in all the cases where no data are available for specifically assessing uncertainty connected to measures.

Uncertainty analysis became a very useful tool for evaluating model reliability and the growing interest of researchers on this topic is demonstrated by the increasing literature production of recent years (among others: Lindblom et al., 2007; Freni et al., 2008; Schellart et al., 2008; Willems, 2008; Deletic, et al., 2009, Dotto et al., 2009; Kleidorfer et al., 2009; Freni et al., 2010). Uncertainty of a model can be represented in two ways: by giving a range (or a band) of values or by providing a posterior distribution of parameter values. The former entails to likely enclose the true value of a specific simulated variable: lower uncertainty is connected with stricter uncertainty bands. Conversely, the latter consists in providing a posterior distribution of parameter values in which the “true” value should be included. Larger bands and more uniform distributions are caused by highly uncertain models. Using the concept of uncertainty, the “best” model is the one able to correctly simulate a specific variable minimising the width of uncertainty bands.

None of the uncertainty analysis methods presented in literature are universally accepted in urban drainage modelling (Freni et al., 2009a). These methods range from classical Bayesian techniques (among others: McCarty et al., 2008; Haydon and Deletic, 2009), to the pseudo-Bayesian ones (among others: Freni et al., 2008b; Thorndahl et al., 2008).

All Bayesian techniques start from prior knowledge regarding the modelling error (that is assumed to reflect a user-selected probability distribution) and parameter distributions thus updating them according to available data by means of Bayes’ theorem application. The most used pseudo-Bayesian technique is the Generalised Likelihood Uncertainty Estimation (GLUE) proposed by Beven and Binley (1992). GLUE neglects any prior knowledge because of the complexity of the model and of the physical system. Bayesian methods are thus conditioned by prior assumptions that have to be verified and may provide unreliable results in terms of final model uncertainty (Freni et al., 2009a). Moreover, the use of transformation functions such as the Box – Cox transformation may reduce the advantages provided by Bayesian methods in the cases where the residuals distribution is skewed.

The present paper is aimed to evaluate the impact of the Box – Cox transformation by verifying different hypotheses and comparing them with the “real” residuals distributions (i.e. without considering Box – Cox transformation. To accomplish such a goal, the uncertainty analysis of a complex integrated urban drainage model was carried out by means of the classical Bayesian method in which Box – Cox transformation is used for correcting the distribution of residuals. In order to evaluate the impact of such transformation, Box – Cox parameter setting was not only based on the evaluation of the residual homoscedasticity (i.e. model residual variances can be transformed in variances that become approximately constant or independent on the model output value) but different values were considered simulating different grades of skewness of the residuals (namely, five different cases were analysed). The Bayesian analysis was compared with the application of GLUE for which the homoscedasticity of residuals is not necessary. The uncertainty analysis developed in this study is mainly based on the principle that, as a common assumption, input data uncertainty, model structural uncertainty and measured uncertainty can be lumped into model parameter uncertainty (Lindblom et al., 2007).

The model has been applied to the Nocella catchment where both quantity and quality data were available.

2. MATERIALS AND METHODS

2.1 The adopted model

In the present study, a bespoke urban integrated model developed during previous studies was applied (Mannina, 2005). The structure of the adopted model will be briefly described here, as the cited literature can be referenced for a more detailed description of the chosen algorithms. The model is able to assess the main phenomena that take place throughout the three components of the integrated system, i.e. sewer system (SS), wastewater treatment plant (WWTP) and receiving water body (RWB). The integrated model is composed mainly of three sub-models for the simulation of the components; each sub-model is divided into a quantity and quality module for the simulations of the hydrographs and pollutographs. The SS was simulated employing the reservoir concept and taking also into account the mechanism of sewer sediment transport therefore including erosion and deposition. The WWTP was modelled straightforwardly taking into account the main

elements that are generally affected by variation of the inflow both in terms of quantity and of quality: the activated sludge tank and the settler. The former was modelled employing a mass balance for the biomass and for the biodegradable substrate whereas the settler was modelled according to the Takács et al. (1991) conceptual modelling approach. Finally, the RWB was modelled considering the simplified form of the Saint Venant equation (kinematic wave) and the advection dispersion equation. A better description of model structure and algorithms can be found in Mannina (2005).

2.2 The adopted case study

The analysis was applied to a complex integrated catchment: the Nocella catchment that is a partly urbanised and partly natural catchment located near Palermo in the north-western part of Sicily (Italy). The entire natural basin is characterised by a surface of 99.7 km², and has two main branches that flow primarily east to west. The two main branches join together at 3 km upstream from the river estuary. The southern branch is characterised by a smaller elongated basin, and receives water from a large urban area characterised by relevant industrial activities partially served by a WWTP, and partially connected directly to the RWB. The northern branch was monitored in the present study. The basin closure is located 9 km upstream from the river mouth; the catchment area is 66.6 km². The catchment end is equipped with a hydro-meteorological station (Nocella a Zucco).

The river reach receives wastewater and stormwater from two urban areas (Montelepre, with a catchment surface equal to 70 ha, and Giardinello, with a surface of 45 ha) drained by combined sewers. Each sewer system is connected to a WWTP protected by CSO devices. The WWTPs are characterised by simplified activated sludge processes with preliminary mechanical treatment units, an activated sludge tank, and a final circular settler. Rainfall was monitored by four rain gauges distributed over the basin: the Montelepre rain gauge is operated by Palermo University, and is characterised by a 0.1 mm tipping bucket and a temporal resolution of 1 minute; the other three rain gauges are operated by the Regional Hydrological Service, and they are characterised by a 0.2 mm tipping bucket and a temporal resolution of 15 minutes. The hydro-meteorological station (Nocella a Zucco) located at the catchment end is characterised by an ultra-sonic level gauge operated by the Regional Hydrological Service, and has a temporal resolution of 15 minutes. The instruments were integrated by Palermo University by installing, for the quantity data, an area – velocity submerged probe that provides water level and velocity data with a 1 minute temporal resolution. An ultrasonic external probe was used to give a second water level measurement for validation, and as a backup in case the submerged probe failed; an automatic 24-bottle water quality sampler was used for water quality data collection. Flow measurements have been carried out using area – velocity probes with 1 minute temporal resolution, which allow the inflow and outflow volumes for each element in the system to be defined. Water quality sampling was performed using automatic 24-bottle samplers.

The monitoring campaign began in December 2006 and is still in progress. Rainfall and discharge were monitored continuously, while water quality was measured during specific periods. Additional details on the catchment and on the monitoring campaign may be found in Freni et al. (2010).

2.3 The uncertainty analysis

The Bayesian method expresses uncertainties in the model parameters in terms of probability. Parameter uncertainty is evaluated starting from a prior probability distribution $P(\theta)$ which represents the historical or expertise information before collecting any new data. The principle of the Bayesian method is to update this prior information using observed experimental data (D) in order to obtain the posterior information. This update is performed using Bayes' theorem, which can be expressed as:

$$P(\theta | D) = \frac{P(D | \theta)P(\theta)}{\int P(D | \theta)P(\theta)d\theta} \quad (1)$$

where the posterior parameter distribution is computed as a function of the prior knowledge $P(\theta)$ of the conditional probability for the measured data given the parameters $P(D | \theta)$ that is often referred to as the *likelihood function* of the model. The general method does not require any hypothesis regarding model error distribution functions; however, when the method is applied, a hypothesis about model error is made to make the method analytically applicable. The most common simplified hypothesis consist in assuming that modelling

errors are homoscedastic. Supposing that residuals between model and observations are distributed according to a normal distribution with null average and variance σ_e^2 , $P(D|\theta)$ can be written in the multiplicative form as:

$$P(D|\theta) = \prod_{i=1}^m \frac{1}{\sqrt{2\pi\sigma_e^2}} \exp\left(\frac{(D_i - Y_i)^2}{-2\sigma_e^2}\right) \quad (2)$$

where Y_i is the modelling response correspondent to the m available measures D_i of a specific variable (i.e. discharges, concentrations, loads, etc.) at a specific system cross-section. Posterior distributions are populated by running Monte Carlo simulations randomly drawing parameter values from prior distributions.

One crucial point for applying this method is the formulation of the likelihood function. If the statistical assumptions for the residual distribution are violated, the results of Bayesian inference are unreliable (Yang et al., 2008). For evaluating the impact of residual heteroscedasticity (i.e. model residual variances is a function of model output value), in the present study a Box–Cox transformation was used (Box and Cox, 1982):

$$y_\lambda = \frac{(y^\lambda - 1)}{\lambda} \quad \text{for } \lambda \neq 0 \quad y_\lambda = \log(y) \quad \text{for } \lambda = 0 \quad (3)$$

where y is any modelling output and λ is the Box – Cox transformation parameter.

On the other hand, regarding the pseudo-Bayesian approach, the GLUE methodology (Beven and Binley, 1992) considers the problem of searching for an optimum parameter set which is converted into a search for sets of parameter values that give reliable simulations. This methodology is attractive because there is no need for detailed distribution functions of the observable variables and of errors when the explicative models provided are complex or the number of parameters is high (Mantovan and Todini, 2006). However, it has to be stressed that such methodology relies on some subjective hypotheses that could prevent its objective application (Freni et al., 2008). Like other Bayesian and pseudo-Bayesian methods, the GLUE method is based on a large number of Monte Carlo simulations, where the random sampling of individual parameters from probability distributions is used to determine a set of parameter values. Parameter sets are compared with respect to their ability to reproduce available observations. Such a comparison is carried out by means of a likelihood measure. The Nash and Sutcliffe efficiency index (Nash and Sutcliffe, 1970) was herein used as likelihood:

$$E = \sum_{k=1}^m \left[w_k \cdot \left(1 - \frac{\sigma_{e,k}^2}{\sigma_{o,k}^2} \right) \right] \quad (4)$$

where $\sigma_{e,k}^2$ is the variance of errors between observed data and simulation results of the k th model variable (discharge, concentrations), $\sigma_{o,k}^2$ is the variance of the observations concerning a specific variables (i.e. discharges, concentrations, loads, etc.) at a specific system cross-section, w_k is the weight of the j th model variable and m is the total number of model variables considered. The likelihood E may assume values in the range $-\infty < E \leq 1$; values close to the unity represent simulations showing small errors while negative values represent poorly behaving simulations. By means of the likelihood measure, parameter sets are thus classified and sets with poor likelihood (with respect to a user-defined threshold) are discarded as “non-behavioural”. All other sets θ_i from behavioural or acceptable simulation runs are retained and their likelihood $E(\theta_i)$ are re-scaled so that their cumulative total sum is equal to 1. The re-scaled likelihood weights $\ell(\theta_i)$ are obtained according to the following equation:

$$\ell(\theta_i) = \frac{E(\theta_i)}{\sum_{j=1}^N E(\theta_j)} \quad (5)$$

where N is the number of retained behavioural simulations. The GLUE approach considers that the distribution of likelihood values is a probabilistic weighting function for the

predicted variables allowing an assessment of the uncertainty associated with the predictions, conditioned on the definition of the likelihood function, of the input data and model structure (Gupta and Shrivastava, 2006). A method for deriving predictive uncertainty bands using the likelihood weights from the behavioural simulations was presented by Beven and Binley (1992). The uncertainty bands are calculated using the 5% and 95% percentiles of the predicted output likelihood weighted distribution. The uncertainty bands should always contain the majority of the observations otherwise the model structure should be rejected. Wider bands mean higher uncertainty in the estimation of the modelling output and thus lower confidence in the model results; vice versa, smaller bands containing the observations are symptoms of reliable and robust modelling approaches.

3. METHODOLOGY APPLICATION

The integrated model was calibrated in previous studies and a sensitivity analysis (considering both quantity and quality model output variables) aimed at reducing the number of model parameters was also carried out (Freni et al., 2010). Parameters were compared by means of the weighted average sensitivity index considering all the RWB modelling outputs simultaneously. Such analysis enabled to reduce the number of significant model parameters from 51 to 37. In the present study, the uncertainty analysis was performed by simultaneously varying the overall influential parameters of the integrated model (i.e. 37 parameters) employing a Monte Carlo approach. The model parameters, their variation ranges and the average model sensitivities are reported in Table 1. Specifically, regarding the average model sensitivities, sensitivity functions have been defined stating the relevance of the dependencies between modelling outputs y and parameters θ :

$$s_{i,j} = \frac{\Delta\theta_j}{y_{s_i}} \frac{\partial y_i}{\partial \theta_j} \quad (6)$$

where $\Delta\theta_j$ is the variability range of parameter θ_j (which depends on prior knowledge) and y_{s_i} is a reference (or scaling) value for the modelling output variable y_i , used for preserving the dimensionless nature of the sensitivity function. The function $s_{i,j}$ is useful because it provides information on the raw dependency of the modelling output on the parameters. The parameters $\Delta\theta_j$ and y_{s_i} , the magnitude and the scaling parameter, respectively, of the sensitivity function, can each have a great influence on the results of the sensitivity analysis (Reichert and Vanrolleghem, 2001). In the present study, y_{s_i} is defined as the average measured value of the i^{th} model output variable, and $\Delta\theta_j$ can be taken as the variation range of the j^{th} model parameter obtained according to single-event model calibrations based on each available rainfall in the calibration dataset (Mannina, 2005; Freni et al., 2010). With multiple modelling outputs, the analysis of the functions $s_{i,j}$ may be only slightly informative and a more aggregated index may be useful. For this reason, a weighted average sensitivity was used for initial parameter evaluation:

$$s_j = \frac{1}{n} \sum_{i=1}^n \frac{s_{i,j}}{\max(s_{i,j})} \quad (7)$$

where $\max(s_{i,j})$ is the maximum of the n sensitivities derived for the j^{th} model parameter.

The model parameters that showed a low influence were highlighted in italic and grey. Parameter variation ranges were assumed as the intervals strictly including the calibrated values obtained by means of all the available monitored events (Beven and Binley, 1992). Both Bayesian and GLUE analysis were based on 1000 Monte Carlo simulations assuming uniform prior distributions for all the parameters. According to the classical GLUE methodology, the user-defined acceptability threshold was set to 0.0 for water quantity and

quality variables. In order to assess the impact of the Box – Cox transformations five cases were considered:

1. CS01: in this case, the value of λ was imposed equal to 1.0;
2. CS02: in this case, the value of λ was imposed equal to 0.5;
3. CS03: in this case, the value of λ was imposed equal to 0.0;
4. CS04: in this case, the value of λ was calibrated by transforming the residual distribution in homoscedastic thus according to the classical Bayesian approach.
5. CS05: in this case, the uncertainty was assessed according to the GLUE methodology.

Table 1 Variation range of model parameters and average model sensitivities (parameters neglected after sensitivity analysis in italic and shaded in grey)

Parameter	Unit	Montelepre			Giardinello		
		Symbol	$\Delta \theta_i$	s_i	Symbol	$\Delta \theta_i$	s_i
Catchment linear channel constant	min	M1	8-30	0.188	G1	1-10	0.221
Initial hydrological abstraction	mm	M2	0.1-04	0.524	G2	0.6-1	0.598
Catchment runoff coefficient	-	M3	0.8-09	0.54	G3	0.6-0.9	0.462
Catchment linear reservoir constant	min	M4	14-40	0.191	G4	0.1-65	0.197
Sewer linear reservoir constant	min	M5	15-35	0.472	G5	0.1-55	0.474
Build-up rate in the Alley-Smith model	kg/(ha*d)	M6	0.1-20	0.307	G6	0.1-20	0.284
Decay rate in the Alley-Smith model	d ⁻¹	M7	0.01-10	0.3	G7	0.01-1	0.225
Wash-off coefficient in the Alley-Smith model	mm ^{-Wh_h(Wh-1)}	M8	0.01-0.8	0.335	G8	0.01-1	0.005
Wash-off factor in the Alley-Smith model (wh)	-	M9	0.3-1	0.24	G9	0.1-3.5	0.437
Sewer erosion factor	kg	M10	0.1-3	0.225	G10	0.1-3	0.341
Sewer suspended load linear reservoir constant	min	M11	0.2-0.8	0.251	G11	0.01-0.6	0.217
Sewer bed load linear reservoir constant	min	<i>M12</i>	0.04-0.4	0.002	<i>G12</i>	0.01-1	0.004
CSO first dilution factor	-	M13	1.2-1.5	0.384	<i>G13</i>	1.1-1.9	0.013
CSO second dilution factor	-	M14	2-4	0.433	G14	2-2.5	0.441
Max yield coefficient of heterotrophs	h ⁻¹	M15	0.6-13.2	0.081	<i>G15</i>	0.6-13.2	0.003
BOD semi saturation constant	g/L	M16	0.005-0.15	0.167	G16	0.005-0.15	0.029
Yield coefficient heterotrophic	-	M17	0.38-0.75	0.225	G17	0.38-0.75	0.032
Temperature	°C	M18	5-30	0.13	<i>G18</i>	5-30	0.014
Max yield coefficient of autotrophs	h ⁻¹	M19	0.2-0.4	0.118	G19	0.2-0.4	0.042
Oxygen half velocity constant	g/L	<i>M20</i>	0.1-0.3	0.001	<i>G20</i>	0.1-0.3	0.002
Yield coefficient autotrophic	-	M21	0.16-0.18	0.428	G21	0.16-0.18	0.226
Decay velocity of heterotrophs	d ⁻¹	<i>M22</i>	0.2-0.8	0.003	<i>G22</i>	0.2-0.8	0.002
Decay velocity of autotrophs	d ⁻¹	<i>M23</i>	0.2-0.8	0.011	<i>G23</i>	0.2-0.8	0.012
		Symbol	$\Delta \theta_i$		s_i		
River bed roughness (Gaukler–Strickler)	m ^{1/3} /s	R1	10 - 70		0.566		
Longitudinal dispersion coefficient	m ² /s	<i>R2</i>	1 - 500		0.001		
De-oxygenation coefficient	s ⁻¹	<i>R3</i>	1 - 100		0.005		
Sediment oxygen demand coefficient	s ⁻¹	R4	1 - 100		0.351		
Re-aeration coefficient	s ⁻¹	R5	1 - 1000		0.894		

4. ANALYSIS OF RESULTS

In the present application, the analysis has been focused on the RWB discharge and quality state. Specifically, with regards to the quantity aspects the RWB discharges at the catchment outlet were considered; whereas for the quality feature, the BOD and DO concentrations at the RWB catchment outlet were taken into account. As outlined in the previous paragraph, in order to assess the impact of the Box - Cox transformation, five different cases were considered: assuming an imposed value of the transformation (CS01, CS02 and CS03), calibrating the best value in terms of homoscedasticity (CS04) and without considering transformations i.e. CS05 (GLUE). Such a comparison was carried out in two ways: by means of parameter posterior distributions and by means of uncertainty bands around the calibrated model outputs. Box – Cox transformation is usually applied after calibrating the residual distribution to be homoscedastic. In the present analysis, for three cases described in the previous paragraph (namely, CS01, CS02 and CS03), Box – Cox transformation was not calibrated in order to investigate the impact of such transformation on the uncertainty analysis results. Conversely, for the case (CS04), λ was calibrated seeking the homoscedasticity of the residual distributions. Specifically, the λ was found equal to 0.512 for the RWB quantity variable (i.e. discharges), 0.497 for RWB BOD

concentrations and 0.493 for RWB DO concentrations. Therefore, CS04, i.e. the results of Bayesian uncertainty analysis after Box – Cox calibration, were considered similar to the case CS02 that assumes $\lambda=0.5$.

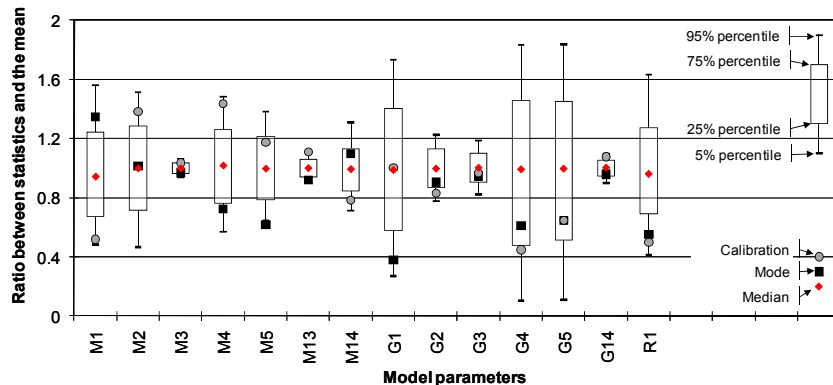
Figures 1 to 4 synthesise the main features of the posterior parameter distributions: the figures show the 5%, 25%, 75% and 95% quantiles of the distributions by means of a box plot; the dots represent some statistics: the mode, the median and the calibration value (all the statistics are referred to the mean value).

Figure 1 shows the characteristics of posterior distribution for the case CS01. More specifically, Figure 1a plots the statistics of model parameters with regards to the quantity aspects (i.e. considering as model output the discharge at the RWB outlet). Conversely, Figure 1b plots the statistics of model parameters with regards to the quality aspects (i.e. considering as model outputs the BOD and DO concentrations at the RWB outlet). The overall characteristics are referred to the mean value for allowing comparison:

- Water quality parameters show larger variability (Figure 1b) than the quantity ones (Figure 1a), and thus higher uncertainties, confirming the frequently expressed consideration in literature that the most part of uncertainty relies in water quality modelling (among others, Freni et al., 2008; Willems, 2008);
- Distribution modes are frequently between 25% and 75% percentiles indicating that the skewness is not high;
- Interestingly, the mode and the calibration value are very close for the case of the some of the most influential parameters. Therefore, there is a model capacity to pin down the value of the most influential parameters in favour of their identifiability. Vice versa, the mode and the calibration values are not superimposed for parameters showing lower influence (low identifiability);
- The median is often near to the mean probably because the posterior distribution is influenced by the prior uniform distribution. Further, the distribution modification during the first Bayesian update, is not relevant.

Figure 2 shows the same results when applying a deeper Box – Cox transformation with a value of λ near the calibration ones (CS02). This case shows the smallest uncertainty among the cases considered in the study. Calibration values are usually included in the range between the 5% and 95% percentile and they are not significantly affected by the transformation apart for some less influential parameters. The impact of transformation on water quality parameters is more relevant, looking at the smaller distance between the 5% and 95%, and it leads to a reduction of perceived uncertainty for them.

Figure 3 plots the case of the most important Box – Cox transformation ($\lambda=0.0$, case CS03). In such a case, for water quantity variables, the parameter distributions become wider reaching levels similar to the case where no transformation is applied. For water quality variables, the case CS03 shows parameter ranges in between the cases CS01 and CS02. This fact may be due to the transformation itself that introduces a deep modification of the modeled and measured time series. Therefore, it reduces the information that may be gathered from the data and thus an increase of the uncertainty of results may take place.



(a)

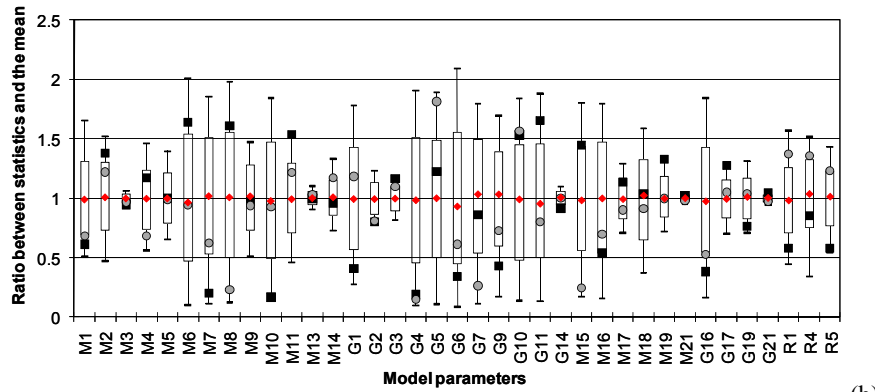


Figure 1 Box plots showing the main characteristics of the parameter posterior distribution applying Bayesian uncertainty analysis with $\lambda=1.0$: (a) quantity model variables and (b) quality model variables.

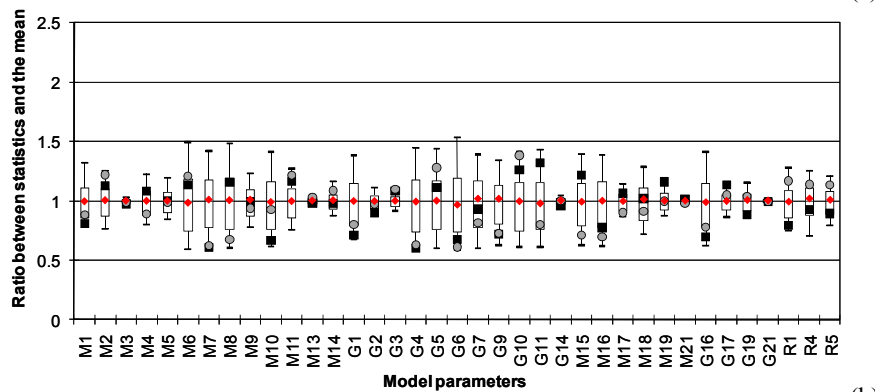
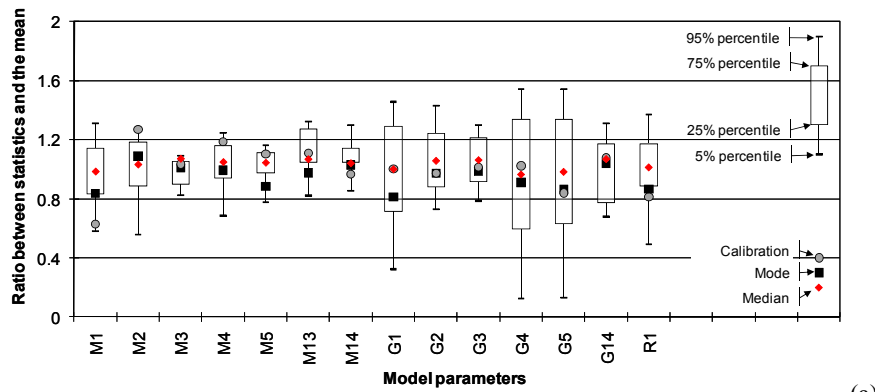


Figure 2 Box plots showing the main characteristics of the parameter posterior distribution applying Bayesian uncertainty analysis with $\lambda=0.5$: (a) quantity variables and (b) quality variables.

Figure 4 shows the statistics with regards to the GLUE case where the uncertainty analysis is carried out without applying transformations and adopting the GLUE approach. Comparing the results of the Bayesian analysis with the GLUE method (based on non-normal likelihood functions), the advantage of the calibrated Box – Cox transformation is evident in gathering more information from the data, thus reducing the perceived uncertainty. Nevertheless, the analysis shows a possible pitfall in the homoscedastic transformation in those cases where residuals are deeply heteroscedastic.

Many parameter distributions in the Bayesian analysis with $\lambda=0.0$ have a width slightly smaller than the GLUE approach showing that the use of formal approaches takes some advantages in terms of perceived uncertainty.

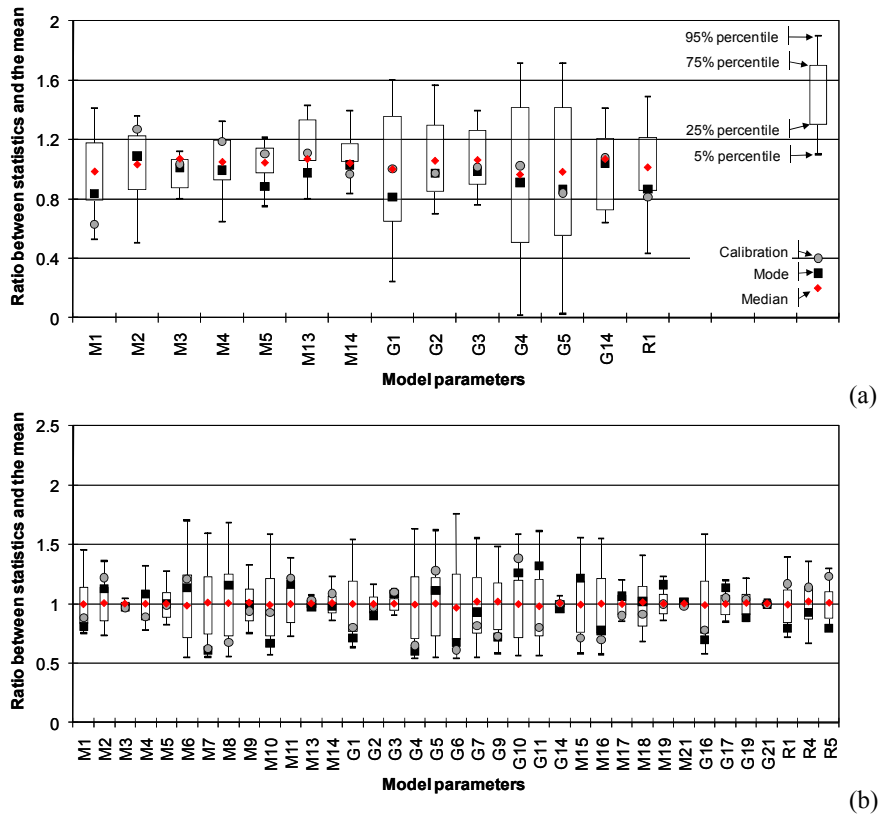
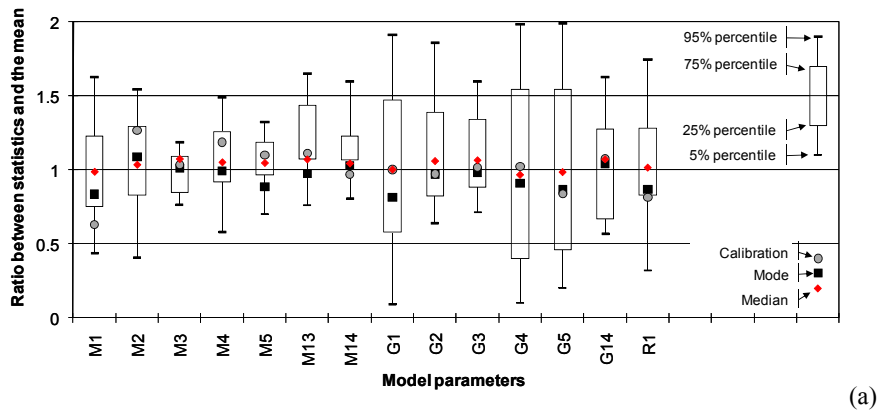


Figure 3 Box plots showing the main characteristics of the parameter posterior distribution applying Bayesian uncertainty analysis with $\lambda=0.0$: (a) quantity variables and (b) quality variables.



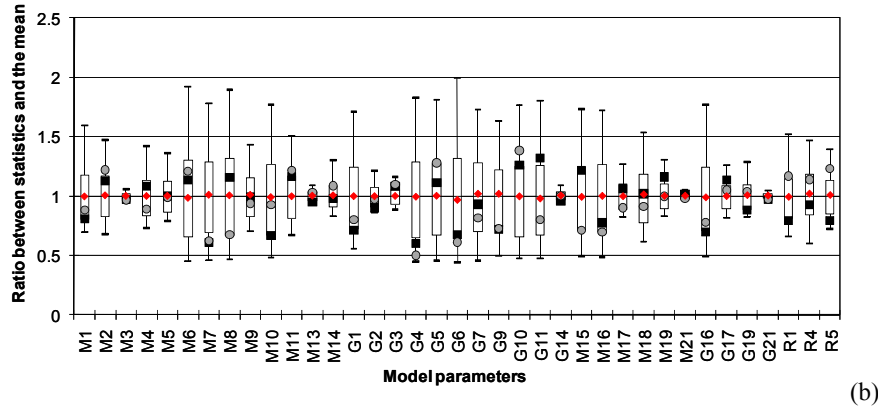


Figure 4 Box plots showing the main characteristics of the parameter posterior distribution applying GLUE uncertainty analysis: (a) quantity variables and (b) quality variables.

Finally, a comparison in terms of uncertainty bands was considered among the five analyzed cases. For the sake of conciseness, in the following only the case CS01 and GLUE are shown as CS03 provided of the Bayesian case without the Box – Cox transformation. Specifically, Figures 5 and 6 show the uncertainty bands, for the case CS03 and GLUE respectively, in the RWB final cross section (Nocella a Zucco) for the analyzed variables: discharge, BOD and DO concentrations. The uncertainty bands obtained by the Bayesian approach with $\lambda=0.0$ are smaller in the average to those provided by GLUE but wider in the regions around the peaks where the effect of the Box – Cox transformation is probably more relevant.

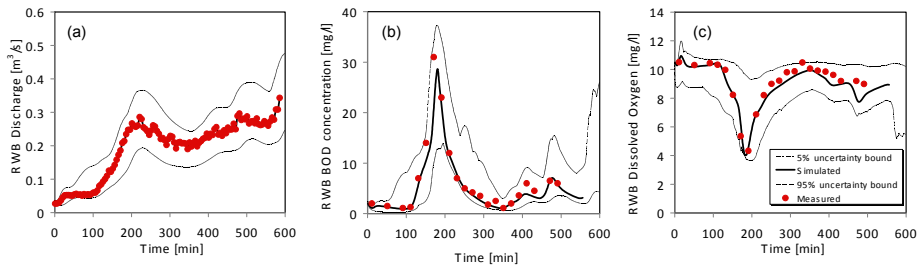


Figure 5 5th percentile and 95th percentile for Bayesian analysis (CS03): (a) RWB discharge; (b) RWB BOD concentration; (c) RWB Dissolved Oxygen.

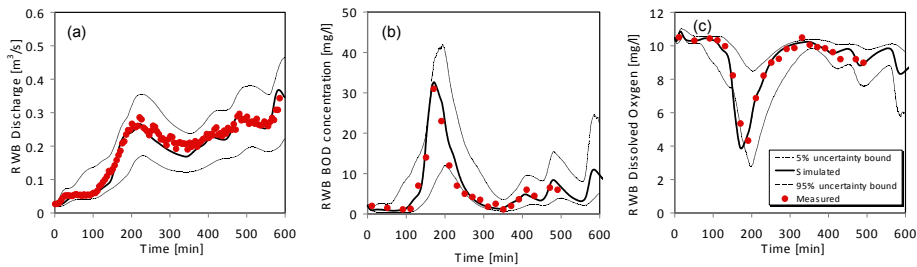


Figure 6 5th percentile and 95th percentile for GLUE analysis (GLUE): (a) RWB discharge; (b) RWB BOD concentration; (c) RWB Dissolved Oxygen.

5. CONCLUSIONS

The paper investigated the impact of Box – Cox transformation that is often applied in Bayesian uncertainty analysis for obtaining homoscedasticity of residuals in complex mathematical models. The transformation modifies the modelled and measured time series and it may interfere with the estimation of uncertainty and its perception by the modeller.

The analysis was carried out by simulating different grades of heteroscedasticity and considering a total of five different cases: three cases by setting the λ value of Box – Cox transformation, a fourth case considering a calibration of λ on the basis of residual homoscedasticity and a fifth case where no transformation of the residuals was considered according to the GLUE methodology. The comparison among the different cases was performed on the basis of two factors: posterior model parameter distribution and uncertainty bands. The analysis showed that the advantages of Bayesian uncertainty evaluation decrease with the increase in residuals heteroscedasticity; model outputs needing deep transformations provide wider posterior parameter distributions and uncertainty bands that are progressively larger even if still smaller than the results of non – formal uncertainty analysis methods (such as GLUE). The analysis of the uncertainty bands shows similar results: the Bayesian approach always provides smaller uncertainty bands even if deeper Box – Cox transformations increases the width of uncertainty bands to the point that, for the case of a λ value ($\lambda=0.0$) and close to the peak value of the simulated variables (discharges, concentrations, load, etc.), they are wider than GLUE. The study showed the importance of the appropriate selection of the uncertainty analysis methodology depending on the specific characteristics of the model and of the real system because a wrong selection of the analysis approach may take to the overestimation of perceived uncertainty.

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