Evaluation of Uncertainty Propagation Predictions in River Water Quality Modeling

André Fonseca (✉ andrerd@gmail.com)

Universidade de Trás-os-Montes e Alto Douro: Centro de Investigação e Tecnologias Agroambientais e Biológicas <https://orcid.org/0000-0001-6792-8047>

Cidália Botelho

University of Porto Faculty of Engineering: Universidade do Porto Faculdade de Engenharia

Rui Boaventura

University of Porto Faculty of Engineering: Universidade do Porto Faculdade de Engenharia

Vitor Vilar

University of Porto Faculty of Engineering: Universidade do Porto Faculdade de Engenharia

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Evaluation of uncertainty propagation predictions in river water quality modeling

André Fonseca^{1*}, Cidália Botelho², Rui A.R. Boaventura², Vítor J.P. Vilar²

¹Centre for the Research and Technology of Agro-environmental and Biological
Sciences – CITAB; Institute for Innovation, Capacity Building and Sustainability of
Agri-food Production – Inov4Agro; Universidade de Trás-os-Montes e Alto Douro,
UTAD, Vila Real, Portugal

²Laboratory of Separation and Reaction Engineering-Laboratory of Catalysis and
Materials (LSRE-LCM), Department of Chemical Engineering, Faculty of Engineering
of the University of Porto, Portugal

*** Corresponding Author**

Tel. +351 936168204; E-mail address: andrerdf@gmail.com (André R. Fonseca)

Abstract

The uncertainty on model predictions to evaluate river water quality is often high to delineate appropriate conclusions. This study presents the statistical evaluation of the water quality modeling system Hydrologic Simulation Program FORTRAN as a tool to improve monitoring planning and mitigate uncertainty in water quality predictions. It also presents findings in determining HSPF model's sensitivity analysis concerning water quality predictions. The computer model was applied to Ave River watershed, Portugal. The hydrology was calibrated at two stations from January 1990 to December 1994 and validated from January 1995 to December 1999. A two-step statistical evaluation framework is presented based on the most common hydrology criteria for model calibration and validation and, a Monte Carlo methodology uncertainty evaluation approach coupled with multi parametric sensitivity analyses to assess model uncertainty and parameter sensitivity. Fourteen HSPF water quality parameters probability distributions are used as input factors for the Monte Carlo simulation. The simulation results for in stream fecal coliform concentrations was found to be most sensitive to parameters that represent first order decay rate and surface runoff that removes 90 percent of fecal coliform from pervious land surface rather than accumulation and maximum storage rates. Regarding oxygen governing process (DO, BOD, NO₃, PO₄), benthal oxygen demand and nitrification/denitrification rates were the most sensitive parameters.

Keywords: Water Resources; Uncertainty Analysis; Sensitivity Analysis; River Water Quality Modeling; HSPF

1. Introduction

Uncertainty in water simulation models is expected due to the difficulty of accurately represent water quantity and quality against a real environment (Beck 1987, van Straten 1998). Extrapolation of water process has proven to be challenging even though there is a thorough knowledge about water process from laboratory experiments. Regardless of the model chosen, great attention must be given when assigning parameters with appropriate and physically meaningful values that accurately describe the watershed in terms of water process through the environment (Doherty & Johnston 2003, Donigian 2002, Fonseca et al. 2014). Because the modeling scale is different from a real environment to a laboratory scale, many model parameters are difficult or impossible to measure. They must often be estimated or evaluated from secondary information sources and are typically laden with notable degrees of uncertainty (Gallagher & Doherty 2007). Evaluating a model performance for observed water quality data hampers the model performance due to data scarcity, accuracy and frequency, since data can be expensive to collect and analyze. Also, water quality data are susceptible to noise and bias due to sampling, handling and measurement procedures (Keith 1990) and often come from sampling programs fixed in frequency and location (Brown & Mac Berthouex 2002). Water quality models are often implemented to investigate the impact of changed boundary conditions on the aquatic system (Wagenschein & Rode 2008) such as sources of pollution that suffer from the same limitations, especially nonpoint sources of pollution are difficult to measure. Compensiously, the lack of good quality data to support model performance is a major cause of model uncertainty.

Sensitivity and uncertainty analysis of model parameters is usually considered one of the primary steps in developing and evaluating models (Jakeman et al. 2006, Sudheer et al. 2011). Over the past decade it has become widely accepted that hydrological models with

numerous parameters are likely to produce equally acceptable predictions for multiple parameter sets (Hope et al. 2004) and a unique “best” parameter set cannot necessarily be found in the parameter space (Christiaens & Feyen 2001). Monte Carlo based methodologies of uncertainty and sensitivity analysis such as those implemented by Hornberger and Spear (1980), Beven and Binley (1992) and Kuczera and Parent (1998) have found myriad applications in environmental modeling, including surface water quality modeling. Uncertainty analysis in environmental modeling can provide information on the “goodness” of a result and enables us to understand the sources of error in the modeling process (Freni & Mannina 2010, Willems 2008). Assessment of the range of uncertainty in model prediction allows decision makers to evaluate the risk when model results are used based on decisions (Novotny & Witte 1997, Reda & Beck 1997), since model outputs from predicting future conditions are somewhat uncertain. An uncertainty analyses attempts to evaluate all possible model outcomes together with their associated probabilities of occurrence, while a sensitivity analyses determines the change in model outputs derived from different model input values.

This paper presents a watershed water quality modelling study in the Ave River watershed (Portugal) to identify those parameters in the selected model, whose accurate characterization is most critical for effective water quality model application. The hydrological model, Hydrologic Simulation Program – FORTRAN (HSPF) was used in this study. HSPF is based on the original Stanford Watershed Model IV and is a consolidation of three previously developed models: Agricultural Runoff Management Model (Moriiasi et al.) (Donigihan & Davis 1978), Nonpoint Source Runoff Model (NPS) (Donigian & Crawford 1976) and Hydrological Simulation Program (HSP) including HSP Quality (Donigian et al. 1991, Donigian Jr et al. 1995). HSPF is a semi-distributed model that simulates water and contaminant transport through spatially distributed, physically

homogenous areas within a watershed called Hydrologic Response Units (HRUs). HRUs are presumed to hydrologically respond similarly to meteorological inputs (precipitation, potential evapotranspiration and temperature). In this way, HSPF can simulate the hydrological, hydraulic and water quality processes on pervious and impervious land surfaces, in soil profiles and streams and well mixed impoundments on a continuous basis (Bicknell et al. 2001, Fonseca et al. 2018, Fonseca & Santos 2019a, b).

2. Materials and methods

2.1. Study area and analysis procedure

Ave River watershed covers an area of approximately 1388 km² located in northern region of Portugal. With a river line of 90.9 km and two main tributaries, Este River (247 km²) and Vizela River (342 km²), it has an annual average precipitation of 1522 mm, an average temperature of 13.9°C and an average annual flow rate of 30.6 m³ s⁻¹. The land use occupation of the basin comprises 46.6% of forest land, 42.6% of agricultural land, 10.7% of urban land and 0.2% of wetland. Meteorological and water quality data for Ave River watershed was retrieved from SNIRH – *Sistema Nacional de Informação de Recursos Hídricos* (National Information System for Water Resources) for the years 1990-2000. A Digital Elevation Model (DEM, 30m) was download from SRTM project (Shuttle Radar Topography Mission) and the Land Use and Soil Data from *Agência Portuguesa do Ambiente- Atlas do Ambiente* (Ministry of Environment, Spatial Planning and Energy). Land use categories were aggregated into 6 main categories (Mapoteca 2008).

The measurement network consists of five meteorological stations, distributed throughout the catchment and two hydrometric gauges, 15E03 (Ave River) and 15E01 (Este River), located 5.3 km upstream the river mouth. The river basin receives several point discharges from industries and wastewater treatment plants. The watershed was delineated to

characterize the stations where observed data was available, station 15E03 Ave River and station 15E01 Este River and segmented according to the meteorological stations (**Figure 1**).

[Figure 1 here]

Using HSPF to simulate water quality requires information about several hydrologic and water quality parameters. Data required by the model included meteorological data, fecal coliform and nutrients loadings from cattle, hogs, wildlife and industry and inflow discharges as time series. Before assessing the model's uncertainty and sensitivity, calibration and validation of flow and water quality parameters were performed. Water quantity and quality of Ave River were calibrated for 1990-1994 and validated for 1995-2000, while Este River was calibrated for 1994-1997 and validated for 1998-2000 (where complete series of observed data was available). For each station concerning quality data, the following parameters were assessed: water temperature, dissolved oxygen (DO), biochemical oxygen demand (BOD), nitrate (NO₃), orthophosphate (PO₄) and fecal coliforms (FC). The calibration and validation plots for all constituents can be found in the supplementary data material (**Figure S1 – Figure S6**).

2.2. Statistical criteria evaluation

To quantify model performance, several statistical measures were calculated for both calibration and validation simulations. Bennett et al. (2013) present several methods for measuring quantitative performance including direct model comparison, comparison of real and modeled values concurrently, key residual criteria, residual methods using data transformations and, correlation and model efficiency performance measures. A brief description of the statistical criteria used follows.

The deviation of runoff volumes, D_v , also known as the percentage bias, is the simplest goodness-of-fit criterion (Legates, et al., 1999). Its value is calculated using the following equation:

$$D_v[\%] = \frac{\sum_i^n (O_i - S_i)}{\sum_i^n O_i} \times 100 \quad (\text{Equation 1})$$

Where,

O_i = observed monthly values for the i^{th} month;

S_i = simulated monthly values for the i^{th} month and:

n = total number of months.

The model simulation performance rating for the deviation of volumes (Donigian Jr. 2002) is considered very good for values inferior to 15%, good between 15 and 25% and satisfactory for values between 25 and 35%.

The Coefficient of Determination (R^2) determines how much a linear fit describes the variance between the two variables. It can vary between 0 and 1, the higher the value the better fit.

$$R^2 = \left[\frac{\sum_{i=1}^n [(O_i - \bar{O})(S_i - \bar{S})]}{[\sum_{i=1}^n (O_i - \bar{O})^2]^{1/2} [\sum_{i=1}^n (S_i - \bar{S})^2]^{1/2}} \right]^2 \quad (\text{Equation 2})$$

Where,

$\bar{O}$ = mean of the observed monthly value;

$\bar{S}$ = mean of the simulated monthly value.

According to Santhi et al. (2001) and Singh et al. (2005) satisfactory model performance is achieved when the coefficient of determination is above 0.6 for monthly simulated constituents, but a value of 0.5 is still acceptable.

The Nash-Sutcliffe coefficient also known as the efficiency criterion (E) is a measure of statistical association, which indicates the percentage of the observed variance that is explained by the model. The Nash-Sutcliffe coefficient is estimated using equation 3:

$$E = 1 - \frac{\sum_{i=1}^n (S_i - O_i)^2}{\sum_{i=1}^n (O_i - \bar{O})^2} \quad (\text{Equation 3})$$

Where $\bar{O}$, is the average measured discharge and all the other variables have the same meaning as mentioned previously. The second term in equation 3 represents the ratio between the mean square error (MSE) and the observed data variance. Thus, if a value of E equals zero it indicates that the model output is not better than the averaged observed streamflow for the entire analysis period. Essentially, the closer the model efficiency is to 1, the more accurate the model is.

The Mean Square Error, MSE, quantifies the difference between values implied by an estimator and the estimated quantity's true value; a value of zero means that the estimator predicts observations of the parameter with perfect accuracy. It can be estimated by using equation 4:

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n (S_i - O_i)^2 \quad (\text{Equation 4})$$

where n is the number of predictions.

The Root Mean Square Error, RMSE, also called the root mean square deviation is the standard deviation of the differences between predicted values by a model and the observed values. The RMSE of a model prediction is defined as (Equation 5):

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n (S_i - O_i)^2} \quad (\text{Equation 5})$$

The Fourth Root Mean Quadruple Error, R4MS4E, is used to put more emphasis on the larger errors by using the fourth power of the RMSE, it can be calculated using equation 6:

$$R4MS4E = \sqrt[4]{\frac{1}{n} \sum_{i=1}^n (S_i - O_i)^4} \quad (\text{Equation 6})$$

The Relative Volume Error, RVE, (Choi et al.) indicates how good measurement is relative to the size of the sample being measured, it can be estimated using equation 7:

$$RVE = \frac{\frac{1}{n} \sum_{i=1}^n (S_i - O_i)}{\frac{1}{n} \sum_{i=1}^n (O_i)} \quad (\text{Equation 7})$$

The Standard Deviation Rati, RSR, same as the RMSE method weighted by the standard deviation of the observed values, can vary between zero and ∞ with an ideal value of zero. It can be estimated using equation 8:

$$RSR = \frac{\sqrt{\sum_{i=1}^n (S_i - O_i)^2}}{\sqrt{\sum_{i=1}^n (O_i - \emptyset)^2}} \quad (\text{Equation 8})$$

Equation 4 through equation 8 values can vary between 0 and ∞ with an ideal value of zero for all criteria.

The Index of Agreement, IoAd, similar to R^2 , is designed to be better at handling differences in modeling and observed means and variances. With an ideal value of 1 it can vary from 0 to 1.

$$IoAd = 1 - \frac{\sum_{i=1}^n (S_i - O_i)^2}{\sum_{i=1}^n (|O_i - \emptyset| - |S_i - \emptyset|)^2} \quad (\text{Equation 9})$$

2.3. Uncertainty and sensitivity analyses

Uncertainty analysis was conducted using a Monte Carlo (MC) approach (Roy & Gupta 2021). Multiple model simulation runs were performed using the 10-year period, with values for the selected model parameters randomly chosen from assigned probability distributions. The water quality parameters that were considered knowledge uncertain are listed in **Table 1** with their respective distributions. The range represents the lower and upper limits for the distributions, which correspond to the typical minimum and maximum limits for these parameters from the HSPF user's manual. Since some parameter values can vary up to infinite, the maximum value used for the distributions was the one observed for the calibrated model. A uniform distribution was assigned to parameters for which no additional information is available in the manual, while accumulation and storage parameters were assigned a triangular distribution where the most probable value is the mode of the calibration model's parameter value. ACQOP and SQOLIM values for the remaining months were calculated by multiplying the January distribution with a monthly adjustment factor from the calibrated model. This result in 14 parameters analyzed.

[Table 1 here]

To ensure that the MC simulations satisfactorily approximate model output uncertainty, 1000 model runs were performed. To calculate the model uncertainty, quantiles of time series weighted by the Nash-Sutcliffe coefficient (E), deviation of volumes (D_v) and the coefficient of determination (R^2), for a 95% confidence interval, were derived for all quality parameters described by (Roy & Gupta 2021). The MC simulations used to generate data for the model comparison were executed using an R script (Team 2008) written specifically for this study. The R script populated all the parameters subroutine tables in the HSPF user control input (UCI) file, resulting in 1000 UCI files representing the distributions' parameter sets.

A multi parametric sensitivity analysis (MPSA) was applied to the parameters referred in **Table 1** to recognize the significance of each parameter involved in the model. The MPSA followed the procedure proposed by Chang andDelleur (1992) and Choi et al. (1998) and consists of implementing a generalized sensitivity analysis (Hornberger &Spear 1981); determine whether the 1000 parameter sets are “acceptable” or “unacceptable” by evaluating the statistical errors mentioned previously; compare the cumulative frequency distributions for each parameter associated with the acceptable and unacceptable results. If the two distributions are not statistically different, the parameter is classified as insensitive, otherwise the parameter is sensitive.

3. Results and discussion

3.1. Model calibration and validation

Simulated and observed daily and monthly flow and stream constituents’ concentration for calibration and validation at Ave and Este River stations were visually compared and evaluated by statistical criteria (**Table 2a, 2b**). The calibration and validation plots for all constituents addressed in this study are provided in the supplementary data material (**Figure S1 – Figure S6**). The statistical criteria were used as a guide in estimating satisfactory model performance. The deviation of volumes values for all constituents produced good results, with fecal coliforms showing the highest deviation at both stations. Nash-Sutcliffe values produced particularly good results for calibration and validation purposes, although nitrates and BOD validation at both stations only revealed a satisfactory approach ($E < 0.50$).

Regarding the coefficient of determination, the constituents that resulted in values inferior to 0.50 (unsatisfactory) were FC, BOD and NO_3 for validation purposes at Ave River station. To prevent the deviation volume effect where positive and negative errors cancel each other, the MSE, RMSE and R4MS4E criteria were calculated. Both criteria show

good results with values close to zero. Although RMSE and R4MS4E are more useful for interpretation since the results returned are in the same units as the model and indicate an overall agreement between predicted and observed data, the bigger the mean square (two to four) the higher the emphasis on larger events. The results indicate that HSPF model is well suited for river discharge simulation and stream water quality in Ave Watershed.

[Table 2a here]

[Table 2b here]

3.2. Uncertainty analysis

The uncertainty analysis was performed for the entire calibration and validation period: 10 years for Ave River station and 6 year for Este River station. The threshold established for the likelihood measure to classify the model parameter sets as acceptable was determined based on the model output for each quality parameter that resulted in positive E values, D_v between -30 and 30%, and R^2 above 0.50, concurrently. Acceptable parameter sets showed E values above 0.40. **Figure 2** and **Figure 3** show the uncertainty band for the water quality constituents addressed in this study with a 95% confidence interval for Ave and Este River respectively.

[Figure 2 here]

[Figure 3 here]

This approach resulted in the number of acceptable parameter sets shown in **Table 3**. Este River station resulted in lesser acceptable parameter sets due to an inferior period of analysis. Nitrate and orthophosphate uncertainty analysis resulted in the lowest acceptable parameter sets observed.

[Table 3 here]

Table 3 also reports the percentage of occurrences in which observed data is within the 95% confidence interval. This shows that the threshold defined as acceptable affects the confidence interval size, also the size of the sample will affect the confidence interval;

Ave River station shows a higher percentage of data within the confidence interval than Este River station, since higher available observed data results in a better calibrated model. When calibrating oxygen governing reactions, the calibrated model will depend on all parameters that will affect nutrients, biochemical oxygen demand and dissolved oxygen. For instance, a good calibration and validation for nitrates do not mean the model describes the watershed perfectly since all other oxygen demanding processes must be analyzed concurrently. From all the acceptable parameter sets, only 32 for Ave River station and 17 for Este River station resulted in behavioral for all oxygen involving processes concurrently for the threshold defined. Changing the threshold of R^2 to 0.40 and D_v limits between -35% and 35% results in 373 and 284 behavioral parameter sets for Ave River and Este River station respectively, with the lowest observed E value of 0.12. Uncertainty analysis of HSPF revealed that the model is unable to capture low values of FC at both stations.

3.3. Sensitivity analysis

The sensitivity analysis for FC output revealed that the model is most sensible to first order decay rate ($FSTDEC$) and the rate of surface runoff that will remove 90% of the store FC ($WSQOP$). The results also show that the maximum storage rate ($SQOLIM$) is more sensible than the monthly accumulation storage ($ACQOP$) (**Figure 4**). The extent of separation between both lines represents the degree of sensitivity of each parameter. **Figure 4** also shows that the sensitive is decreased with the increase of observed data and therefore a better model fit, but both sensitivity analysis (Ave River and Este River) confirmed the same parameters as the most sensitive in the model.

[Figure 4 here]

Dissolved oxygen concentration was more sensitive to benthal oxygen demand ($BENOD$) and nitrate denitrification rate ($KNO320$), nitrates were more sensitive to the rate of

removal of nitrogen storage (*WSQOP*), nitrification rates (*KNO320* and *KNO220*) and the biochemical oxygen demand rate (*KBOD20*) at both stations. Regarding orthophosphorus, all parameters analyzed showed similar cumulative frequencies, though the surface runoff rate of phosphorus (*WSQOP*) and benthal oxygen demand (*BENOD*) were the most sensitive parameters for calibration orthophosphates at both stations. Biochemical oxygen demand parameters sensitivity were governed by almost all parameters analyzed but the more significant ones were the decay rate (*KBOD20*) and the settling rate (*KODSET*) at Este River station, where at Ave River station no parameter showed a significant degree of sensitivity. This means that all parameters are to be considered important when calibrating biochemical oxygen demand concentration. **Figure 5** shows the frequency distributions of the most sensitive parameters addressed here.

[Figure 5 here]

The oxygen governing process involves many parameters to perform a proper calibration of the model (Man et al. 2021). While MPSA does not show a top sensitive parameter, some could be considered of great importance. The results show that biochemical oxygen demand decay rate (*KBOD20*), nitrification rates (*KNO320* and *KNO220*) and benthal oxygen demand (*BENOD*) are key parameters for good model calibration. Accumulation rates (*ACQOP*) and maximum storage (*SQOLIM*) of nutrients did not result in high output variation, though the results may be masked by the rate of removal of nutrients (*WSQOP*) that simulates the wash off of nutrients from the land. Further, algae simulation parameters, such as phytoplankton growth and settling rates should be considered, however no observed data was available at any of the stations, which made it impossible to perform a calibration and statistically classify it as acceptable or unacceptable.

4. Conclusions

Uncertainty in water quality modeling is usually high due to data scarcity. The complexity of the model approach (high parameterization) and the likelihood established greatly modify the propagation of uncertainties, especially with the uncertainty associated with limited quality data. Without good calibration data (or scarce), it is especially hard to validate a model. Despite this, water quality models are an important tool to assist managers in modeling a complex system. An uncertainty and sensitive analysis can lead to additional resources being made available for future management and monitoring, by providing vital information to improve budget allocation for both target assessment (more accurate quality data) and eventually reduce uncertainty in model results. The results obtained from this study can be used to direct future efforts in collecting more information that would help to characterize the most sensitive parameters and those subject to more significant uncertainty.

The results of this paper can provide references for parameter calibration of water quality prediction using HSPF. The main findings are summarized below:

- High sampling is needed to get representative samples for a specific site; Este River station parameters uncertainty resulted in narrower confidence intervals than Ave River station due to data scarcity which led to inferior acceptable parameter sets;
- Two parameters, *FSTDEC* followed by *WSQOP*, have a great influence on FC concentration model output;
- Accumulation and maximum storages of nutrients are less important than kinetic governing equations for nutrient calibration;
- At the same time the high parameterization of the integrated model does not allow for clearly identifying relevant parameters, especially to oxygen governing processes where several parameters show similar behaviors on modeling outputs;

These results are partly subjective and will depend on the specific details of watersheds, though they can be extrapolated to similar behavioral watersheds with strong agricultural emphasis. Nonetheless, the results provide a general guide to reduce uncertainty when modeling water quality constituents.

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Figures

Legend

- Hydrometric Stations
- Meteorological Stations
- Streamline
- Ave Sub Basins
- Segment 05F02
- Segment 05G05
- Segment 05G03
- Segment 05H01
- Segment 04I01
- Segment 04H02

Figure 1

The measurement network consists of five meteorological stations, distributed throughout the catchment and two hydrometric gauges, 15E03 (Ave River) and 15E01 (Este River), located 5.3 km upstream the river mouth. The river basin receives several point discharges from industries and wastewater treatment

plants. The watershed was delineated to characterize the stations where observed data was available, station 15E03 Ave River and station 15E01 Este River and segmented according to the meteorological stations. Note: The designations employed and the presentation of the material on this map do not imply the expression of any opinion whatsoever on the part of Research Square concerning the legal status of any country, territory, city or area or of its authorities, or concerning the delimitation of its frontiers or boundaries. This map has been provided by the authors.

Figure 2

The uncertainty analysis was performed for the entire calibration and validation period: 10 years for Ave River station and 6 year for Este River station. The threshold established for the likelihood measure to classify the model parameter sets as acceptable was determined based on the model output for each quality parameter that resulted in positive E values, Dv between -30 and 30%, and R2 above 0.50, concurrently

Figure 3

The uncertainty band for the water quality constituents addressed in this study with a 95% confidence interval for Ave and Este River respectively.

Figure 4

The sensitive is decreased with the increase of observed data and therefore a better model fit, but both sensitivity analysis (Ave River and Este River) confirmed the same parameters as the most sensitive in the model.

Figure 5

The frequency distributions of the most sensitive parameters addressed here.

Supplementary Files

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