SENSITIVITY AND UNCERTAINTY ANALYSIS FOR RIVER WATER QUALITY MODELLING

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ABSTRACT

Uncertainty analysis for model simulations is assuming a growing importance in the field of water quality management. The importance of this concern is provided by recent public awareness over health risks from improper disposal of toxic wastes as well as by the continuing emphasis on risk assessment. The first step in the chain of the risk assessment is the quantification of the error in predicting water quality. For each mathematical modelling application, different uncertainties are involved. The uncertainty-sources can be classified into different categories (model-input uncertainty, model-structure uncertainty, model-parameter uncertainty and measurement errors). These different types of uncertainty sources determine collectively the total uncertainty in the model results. In this paper, the relative contributions of uncertainties associated with each source were studied. This provides information as to where available resources should be focused.

Keywords: Sensitivity analysis, uncertainty analysis, Monte Carlo simulation

INTRODUCTION

Mechanistic modelling of physical systems is often complicated by the presence of uncertainties. Environmental and biological modelling, for example, entails uncertainties in the estimates of toxicant emissions, transformation and transport parameters, etc., that impact the estimates of related health risks. The implications of theses uncertainties are particularly important in the assessment of several potential regulatory options, for example, with respect to the selection of a strategy for the control of pollutant levels.

The purpose of quantitative uncertainty analysis is to use currently available information in order for quantifying the degree of confidence in the existing data and models. In fact, it is precisely for problems where data are limited and where simplifying assumptions have been used that a quantitative uncertainty analysis can provide an illuminating role, to help identify how robust the conclusions about model results are, and to help target data gathering efforts (Frey, 1992). For each mathematical modelling application, different uncertainties are involved. The uncertainty-sources can be classified into the following categories: uncertainties of the model input variables (input uncertainties), uncertainties of the model parameter values (parameter uncertainties), uncertainties originating from the imperfect description of the physical reality by a limited number of mathematical relationships (model–structure uncertainties) and uncertainties of the measurements (measurement uncertainties).

The primary objective of the sensitivity and uncertainty analysis in this research paper is to study the uncertainties associated with each of the above mentioned uncertainty sources. Further, this can be used to identify the relative contributions of uncertainties associated with each source. This provides information as to where available resources should be focused, for example, increasing the amount of input data to calibrate the model parameters, filling data gaps, through having more detailed measurement campaigns or refining the model used for the problem.

PROBABILISTIC APPROACH FOR UNCERTAINTY ANALYSIS

Different uncertainty types

For each mathematical modelling application, different uncertainties are involved. Willems (2000) stated that this classification into different types is based on the different physical nature of the uncertainties and the model entities to which the uncertainties are related. Model input, model parameters and model structures indeed have a very different physical nature. Model input consists of directly measured data or is estimated. For water systems, they are essentially variable in time. This is opposed to model parameters, which are considered as constant properties, and for which the values are measured, estimated or calibrated. The model structure is assumed on the basis of scientific knowledge (from previous research) or is built on the basis of data available for the model-output variables. Also the mathematical relationships of the model structure are considered fixed and do not vary in time.

REPRESENTATION OF UNCERTAINTIES BY STOCHASTIC TERMS

In a probabilistic model, the different uncertainty sources can be represented by so-called 'stochastic terms'. These terms take the form of random variables E, which are random in magnitude and time. The randomness in the magnitude is described by probability distributions, while the randomness in time is represented by autocorrelations of the time series. To transform the deterministic mathematical model into a probabilistic one, the stochastic terms E_X are added to the model variables x to which the probability distributions are related. In this way, the stochastic term represents an absolute error for the variable X.

APPLICATION TO MOLENBEEK CASE STUDY

The probabilistic methodology has been applied to the physico-chemical water quality modelling of the Molenbeek brook in Belgium. The Molenbeek brook is one of the main tributaries of the River Dender basin, and is located in the Flemish region of Belgium to the west of Brussels. It has an area of 57.44 Km^2 and one liminigraphic station (hourly water level measurement and rating curve) is available at Mere with an upstream area of 40.5 Km^2 (see Figure 1.1). It is a narrow catchment with relatively steep slopes. The upstream part is rural, while the downstream part is more urbanized (villages of Mere, Erpe and Hofstade). For this river, a Mike 11 model (DHI) has been implemented before for the conceptual hydrological modelling, hydrodynamic modelling and physico-chemical water quality (WQ) modelling. Details about this modelling can be found in Radwan (2001). The aim is to separate the total uncertainty (total deviation between model results and measurements) in terms of the variance into the following terms:

$$\sigma^2_{Total} = \sigma^2_{HY+HD} + \sigma^2_{WQ} \tag{1}$$

$$\sigma^2_{WQ} = \sigma^2_{model-input-unc.} + \sigma^2_{model-parameters-unc.} + \sigma^2_{model-structure-unc.} + \sigma^2_{measurements-errors} \tag{2}$$

in which:

σ^2_{Total}	Total uncertainty,
σ^2_{HY+HD}	Hydrological and hydrodynamic modelling uncertainty,
σ^2_{WQ}	Water quality (WQ) modelling uncertainty,
$\sigma^2_{model-input-unc.}$	WQ model input uncertainty,
$\sigma^2_{model-parameters-unc.}$	WQ model parameter uncertainty,
$\sigma^2_{model-structure-unc.}$	WQ model structure uncertainty and
$\sigma^2_{measurements-errors}$	WQ measurements errors.

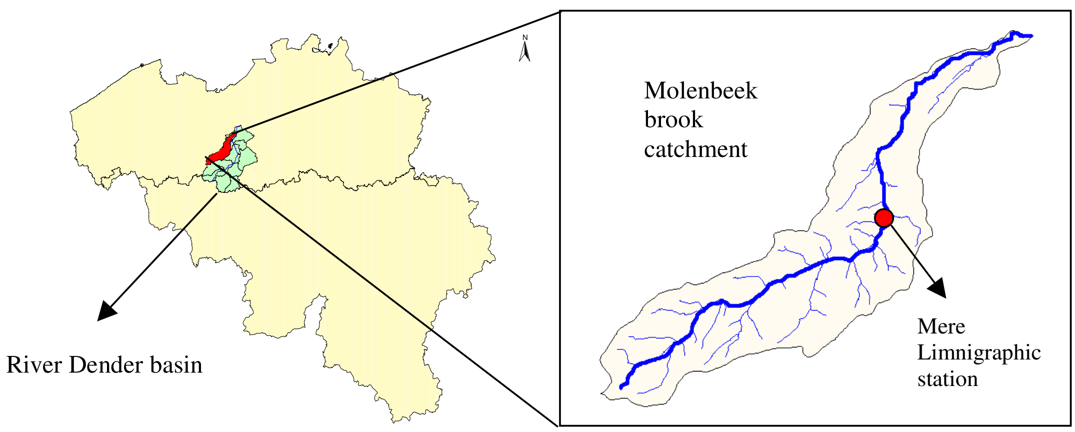

Figure 1 Plan view of the Molenbeek brook catchment, together with the localization within the larger river Dender basin and Belgium.

First, the total uncertainty is quantified, whereafter the other uncertainty-types are estimated as subcomponents of this total uncertainty.

TOTAL UNCERTAINTY

The total uncertainty is estimated after comparison of the Mike 11 simulation results, as described in Radwan (2001) with the WQ measurements as follows:

$$\sigma^2_{total} = \frac{\sum_{i=1}^{n} (x_{Mike11,i} - x_{measured,i})^2}{n-1} \tag{3}$$

where:

$x_{Mike11,i}$: Mike 11 results for the time moments, for which WQ measurements $x_{measured}$ are available. In total n measurements are used (i = 1,….,n).

The results of these σ calculations are given for different WQ parameters. Then a random (Monte Carlo) simulation is performed with a stochastic terms E_{BOD}, E_{DO}, $E_{NH4\text{-}N}$ *and* $E_{NO3\text{-}N}$. Using a moving average technique, the relation of the standard deviation with x can be quantified. This relation can be calibrated well, and is used on the basis of the stochastic terms to describe the average total uncertainty:

$$\sigma^2_{BOD} = (0.046BOD + 0.7459)^2 \qquad \sigma^2_{DO} = (0.254DO - 0.3967)^2 \tag{4), (5}$$

$$\sigma^2_{NH_4-N} = (0.0932NH_4 - N + 0.7502)^2 \qquad \sigma^2_{NO_3-N} = (0.3202NO_3 - N - 0.1166)^2 \tag{6), (7}$$

UNCERTAINTIES FROM HYDROLOGICAL AND HYDRODYNAMIC MODELLING

The results from the hydrological (HY) simulation are used as input for the hydrodynamic (HD) simulations. Finally the results from the HD are used as input for the water quality simulations. To determine the contribution of the hydrological and the hydrodynamic uncertainties to the total uncertainty, the standard deviation of the difference between the HY and HD simulation results and the river discharge measurements is calculated. Then a random (Monte Carlo) simulation is performed with a stochastic term E_{HY+HD}. Using a moving average technique, the relation of the standard deviation with x can be quantified. Also this relation can be calibrated well, and represents the average contribution of the HY+HD models in the total uncertainty:

$$\sigma^2_{HY+HD(BOD)} = (0.0096BOD + 0.5)^2 \qquad \sigma^2_{HY+HD(DO)} = (0.1)^2 \tag{8), (9}$$

$$\sigma^2_{HY+HD(NH_4-N)} = (-0.0002NH_4 - N + 0.8)^2 \qquad \sigma^2_{HY+HD(NO_3-N)} = (0.05)^2 \tag{10), (11}$$

TOTAL WATER QUALITY MODEL UNCERTAINTY

After computation of the contribution of the uncertainty of the hydrological and hydrodynamic input to the water quality model, the remaining range is explained by the water quality modelling. The uncertainty due to the water quality modelling can be splitted into the different uncertainty sources (subgroups). In the following sections, the detailed calculations of each subgroup are presented.

WATER QUALITY MODEL-STRUCTURE UNCERTAINTY

For different water quality models, the water quality process equations are describing the changes in the constituent concentrations due to biological, chemical, biochemical and physical processes. To be able to quantify the uncertainties due to the model structure, different model-structures have to be compared. In this study, the Mike 11 water quality module (DHI, 1993) is compared with Qual2E (Brown and Barnwell, 1987). The process formulations of both river water quality models are similar. In spite of this general similarity, there are some remarkable differences. Examples of these differences are:

- The simplified treatment of nitrification in Mike11 that ignores nitrite as an intermediate product.
- Inhibition of nitrification at low dissolved oxygen concentration is considered only in the Qual2E model.
- Fraction of Algal uptake from nitrogen pool is considered only in the Qual2E model
- Denitrification process is considered in the Mike 11 model and not in the Qual2E model
- Algae is not considered in the DO cycle in Mike 11

The difference between the two models is calculated as the variance between the simulation results of the two models. The difference between the concentration results for the two models show no dependency with the concentration, so the model structure uncertainty can be written as follows:

$$\sigma^2_{model-structure-unc.(BOD)} = (0.206)^2 \qquad \sigma^2_{model-structure-unc.(DO)} = (0.148)^2 \qquad (12), (13)$$

$$\sigma^2_{model-structure-unc.(NH_4-N)} = (0.036)^2 \qquad \sigma^2_{model-structure-unc.(NO_3-N)} = (0.02)^2 \qquad (14), (15)$$

Water quality measurements uncertainty

The measurement errors found in the literature (Ahyerre et al., 1998) are 15 % - 20 % for most water quality variables and 30 % - 40 % for BOD. For these values, half of the error can be explained due to sampling and the other half due to the analysis technique in the laboratory. For BOD, the laboratory analysis has a larger contribution (Willems, 2000).

INPUT AND MODEL PARAMETER UNCERTAINTY

On the basis of the analysis of parameter uncertainty, a sensitivity analysis can be used. With such an analysis, the parameters that have the greatest effect on the model output can be identified. The effort involved in gathering data to characterize the uncertainty in each parameter is considerable so the sensitivity analysis helps to focus on parameters most important for model calibration.

To try to split the range to uncertainties due to model parameters and uncertainties due to model input, the sensitivity of each model parameter and model input change to the model output response is studied. The sensitivity of each term can be calculated as a percentage of the total variance. For example, for DO the sensitivity of the nitrification process rate k_{nitr} is calculated as follows:

$$S_{k_{nitr}} = \frac{\sigma^2_{k_{nitr}}}{\sigma^2_{model\_input+model\_parameter(DO)}} \tag{16}$$

The results of the sensitivity analysis show that, in general, model input is more sensitive than model parameters. For DO, BOD, NH_4-N and NO_3-N the percentage of the model input sensitivity to the sum of model input and model parameter sensitivity is 58%, 93%, 94.5% and 79% respectively.

After having an idea about the sensitivity of each of the model input and parameters, a random error is estimated according to the experience of the author in combination with the available literature. For example, the ranges (standard deviation) for nitrification, denitrification and BOD decay process rates values are adapted from Van der Perk, (1996). The dependency in time of the random errors modelled by the stochastic term is represented by an autocorrelation model. The most flexible model structure for this autocorrelation model is the ARMA structure [Willems, 2000]. After running the random (Monte Carlo) simulations by taking into account the random errors and the correlation as mentioned above, results are derived for the standard deviation of each parameter and model input. An example of such results is shown in Figure 1.2 for DO.

CONCLUSION

In water quality models for water resources management and planning, the model output depends on the input data and a number of parameters that are essentially stochastic processes or random variables. The task of the uncertainty analysis is to estimate the different uncertainty contributions to the model output in terms of the uncertainties in the input, the model parameters and the model structure. Also the measurement errors have to be taken into account. The results of the Monte Carlo simulation show that, the percentage of model input contribution to the total uncertainty is 61 % for DO, 56% for BOD, 56% NH_4-N and 72% for NO_3-N. For the percentage of the contribution of model parameters to the total uncertainty, values of 37% for DO, 31% for BOD, 37% for NH_4-N and 24% for NO_3-N are derived. Finally, the model structure uncertainty contribution to the total uncertainty is 2% for DO, 13% for BOD, 7% for NH_4-N and 4% for NO_3-N. When water quality model results are compared with measurements, part of the deviation can be explained by measurement errors: 2% for DO, 20% for BOD, 17% for NH_4-N and 15% for NO_3-N. From the previous results, it is clear that the model input need most attention to better assess their values. Model parameters and model calibration needs second most attention, followed by the measurement accuracy. Finally, the model structure needs less attention as it contributes only with a small percentage to the total uncertainty (in this study however only analysed by comparing the Mike11 and Qual2E model structures).

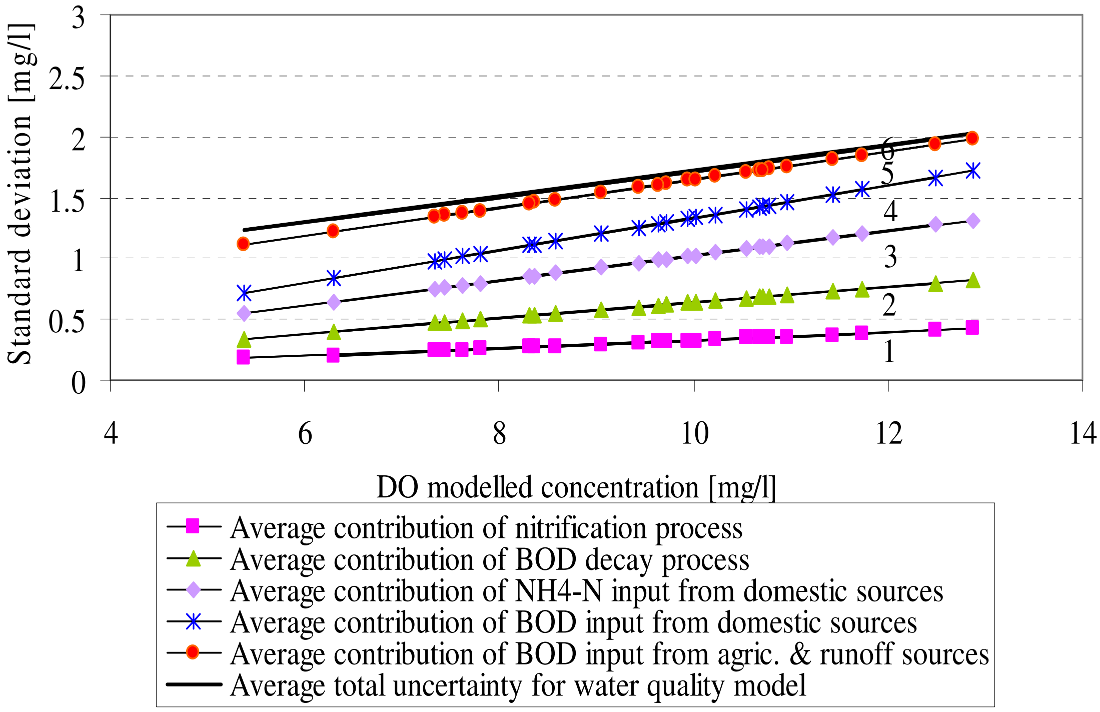

Figure 2 Average total uncertainty for the DO model with the average contribution of 1) nitrification process, 2) BOD decay process, 3) NH4-N input from domestic sources, 4) BOD input from domestic sources, 5) BOD input from agricultural & runoff sources, 6) model structure and measurements uncertainty.

REFERENCES

1. Ahyerre, M., Chebbo, G., Tassin, B., and Gaume, E. Storm water quality modelling, an ambitious objective?, *Water Science and Technology*, Vol. **37**, No. 1, 205-213.
2. Brown, L.C. and Barnwell, T.O. (1987). The enhanced stream water quality models Qual2E and Qual2E-uncas: Documentation and user manual, report EPA/600/3-87/007, U.S.EPA, Athens, GA, USA.
3. Danish Hydraulic Institute (DHI), 1993. MIKE11, A microcomputer-based modelling system for rivers and channels, User & reference manual, Version 3.1, DHI, Horsholm, Denmark.
4. Frey, H.C., Quantitative analysis of uncertainty and variability in environmental policy making. Available from: Directorate for Science and Policy Programs, American Association for the Advancement of Science, 1333 H Street, NW, Washington, DC, September 1992.
5. Radwan, M., Willems, P., El-Sadek, A., and Berlamont, J., (2000). Water quality modelling as an environmental issue. International conference on Water resources management 2001, Halkidiki, Greece, 24-26 September 2001, 185-194.
6. Van der Perk, M. Uncertainty issues in modelling the influence of bed sediments on water composition, Ph.D. thesis. Koninklijk Nederlands Aardrijkskundig Genootschap, Utrecht, Faculteit Ruimtelijk Wetenschappen unversiteit Utrecht.
7. Willems, P. (2000). Probabilistic emission modelling of receiving surface waters, Ph.D. thesis, Catholic University of Leuven, Belgium.