

# Application of MCMC – Global Sensitivity Analysis Method for Model Calibration to Urban Runoff Quality Modeling

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**Abstract:** In stormwater quality modeling, estimating the confidence level in conceptual model parameters is necessary but difficult. The applicability and the effectiveness of a method for model calibration and model uncertainty analysis in the case of a four parameters lumped urban runoff quality model are illustrated in this paper. This method consists of a combination of the Metropolis algorithm for parameters' uncertainties and correlation assessment and a Variance-based method for global sensitivity analysis. The use of the Metropolis algorithm to estimate the posterior distribution of parameters through a likelihood measure allows the replicated Latin Hypercube Sampling method to compute the parameters' importance measures. Calibration results illustrate the usefulness of the Metropolis algorithm in the assessment of parameters' uncertainties and their interaction structure. The sensitivity analysis demonstrates the insignificance of some parameters in terms of driving the model to have a good conformity with the data. This method provides a realistic evaluation of the conceptual description of the processes used in models and a progress in our capability to assess parameters' uncertainties.

**Keywords:** Uncertainty analysis, Global sensitivity analysis, Bayesian inference, Model calibration, Urban runoff, Quality modeling

## 1. INTRODUCTION

Since the seventies, an important number of research programs (National Urban Runoff Program, in the USA (1978-1983), French Campaign (1980-1982), Experimental Urban Catchment “le Marais” (1994-2000), ...) have shown that the urban stormwater is a significant source of pollution for the receiving systems. This pollution results mostly from the erosion caused by the runoff of particulate pollutants accumulated on the urban surfaces and in sewers during the dry weather period (Figure 1). Moreover, in old urban centers combined<sup>†</sup> sewer systems are found, whereby, during wet weather periods, mixed rain and wastewaters may reach the receiving system through combined sewer overflows.

Within the European Union, control of this pollution was concretized in government policy and Community legislation. Concerning the urban drainage, the European Directive n°91/271 of May 1991 on wastewater treatment forces the communities to take into account the pollution discharged into receiving waters during storm events.

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<sup>†</sup> Combined sewer system is used in old cities to drain both the urban stormwater and the wastewater

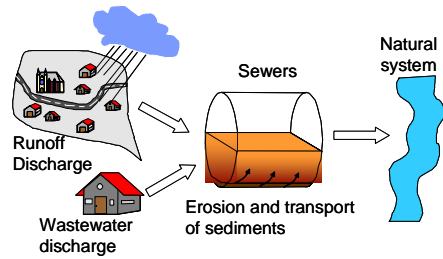


Figure 1 Sources of urban water pollution

Mathematical and computational modeling seems to be a necessary decision-making tool for the management of urban stormwater pollution. Currently, existing models are based on a combination of complex models including conceptual but empirical formulations that describe the processes of generation and transport of pollutants during rainfall. The parameters governing these functions do not have a physical interpretation and therefore, cannot be measured directly in the field. Instead, these parameters must be indirectly estimated using a calibration procedure whereby the model's parameters are adjusted until the system's and the model's outputs show an acceptable level of conformity.

However, the difficulty, expensiveness and uncertainty level of the in situ measurement of urban stormwater pollution generate data that rarely allow a satisfactory calibration and validation of these models [1]. Furthermore, classical optimization methods that are still used up to date for calibration don't allow neither an estimation of the significance of the obtained optimal parameter set, nor a realistic quantification of models' uncertainty. Thus, the existing urban stormwater quality models are rarely used for practical application.

In this paper, we present the results of testing the applicability and the effectiveness of a method for model calibration/validation/sensitivity analysis in urban runoff quality modeling. This method based on the Monte Carlo Markov Chain sampling techniques "MCMC" consists of a combination of a Metropolis algorithm for statistical inference and a Variance-based method for the Global Sensitivity Analysis. This test will be done using data resulting from a survey conducted on the «Marais» catchment in the center of Paris – France [2].

This paper is organized as follows: In section 2, we discuss the difficulties encountered in urban runoff quality modeling. In section 3, we present a general overview of the uncertainty and sensitivity analysis methods. In section 4, we describe the MCMC-GSA method by introducing the Metropolis algorithm, the replicated Latin Hypercube sampling method and their use in the model's calibration and sensitivity analysis. In section 5, we examine the applicability of this method in the case of urban runoff quality modeling. Finally, in section 6, we summarize the methodology and discuss the results.

## 2. URBAN RUNOFF QUALITY MODELING

It is obvious that modeling represents a necessary tool for understanding the behavior of the urban drainage system and a predictive tool in decision making. For this purpose, models have been developed to simulate the urban water cycle for both quantitative and water quality aspects. Concerning quantitative stormwater management, researchers developed runoff and water flow models that are widely used by managers. However, concerning storm water quality management, researchers built complex models whose structure corresponds to the course of pollution. These models simulate the pollutants' accumulation on the urban catchments, their erosion by runoff, the erosion of sediments in the sewers, and finally the

transport of pollutants through sewers to the outlet. However, despite that many models have been proposed since 1971 (first version of SWMM by US-EPA), several difficulties are facing attempts of stormwater quality modeling.

First of all, the physical, chemical and biological phenomena occurring simultaneously at each stage of the processes of generation and transport of pollution in the system make the system very complex. Moreover, space scales vary greatly considering the heterogeneity of the system's characteristics (topography, watersheds, pipes, sediments size), and time scales vary from several days corresponding to the dry weather period, to few minutes during the wet weather period. Therefore, the only possible modeling approach is the conceptual one.

Second, despite the efforts that have been done to understand the sources and the mechanisms governing the processes involved, the dynamics of accumulation, erosion and transport of pollutants are not well known especially in what concerns the sources and processes of pollution generation in sewers. Currently, modelers tend to divide the urban catchment to a number of sub-catchments of few tens of hectares connected by a sewer network. Runoff models, which are initially developed for surfaces, are used to conceptually describe the accumulation and erosion processes on sub-catchments for which little knowledge is currently available. Erosion and transport models of in-sewers solids' are derived from alluvial hydrodynamics, which poorly describe the real behavior of a sewer system during a rain event. So, great discrepancies exist between the current state of knowledge concerning phenomena and the models used.

Third, field surveys for collecting data necessary for the development of models are difficult and expensive. In consequence, input data (topography, sediment sewer deposits, rain intensity, etc...) and quality measurement data (pollutants concentrations) are rare and characterized by great uncertainties (in the range of 30%) [1]. They rarely allow a satisfactory calibration of the model's parameters.

Finally, while considerable attention has been given to develop global calibration procedures that estimate a best set of parameter values, noting that this is not an easy task especially that most of the models are non-linear [3, 4], much less attention has been given to both the assessment of the significance of the obtained optimal set of parameters, and the realistic quantification of models' uncertainty. Thus the estimated parameters from these models are generally error-prone leading to considerable uncertainty in the calibrated model.

Improving these models and their usefulness requires modelers to use a more robust methodology for calibration and validation of models. Such methodology should be able to provide both an assessment of the uncertainties in the model's parameter values and an evaluation of the confidence level of the model's predictions. Uncertainty and sensitivity analysis are therefore indispensable for any modeling improvement attempt in this field.

### **3. UNCERTAINTY AND SENSITIVITY**

In the last decade, great attention has been given to the Bayesian inference for model calibration and uncertainty assessment particularly in the case of complex hydrological models [5, 6]. Nevertheless, its application in environmental modeling is very rare.

Bayesian approach, expresses uncertainties in the model's parameters  $\theta$  in terms of probability. Parameter uncertainty is quantified first by introducing a prior probability distribution  $P(\theta)$ , which represents the knowledge about  $\theta$  before collecting any new data, and

second, by updating this prior probability on  $\theta$  to account for the new data collected ( $D$ ). This updating is performed using Bayes' theorem, which can be expressed as:

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

Where  $P(\theta|D)$  is the posterior distribution of  $\theta$ ,  $\int P(D|\theta) \cdot P(\theta) \cdot d\theta$  is a normalizing constant required so that  $\int P(\theta|D) \cdot d\theta = 1$ , and  $P(D|\theta)$  is the conditional probability for the measured data given the parameters.  $P(D|\theta)$  is often referred to as the likelihood function.

Unlike traditional statistical theories based on first order approximations and multi-normal distributions that may fail especially when dealing with nonlinear complex models [5], Monte Carlo Markov Chain "MCMC" technique have become increasingly popular as a general method that provides a solution to the difficult problem of sampling from a high dimensional posterior distribution [7]. The idea behind MCMC for Bayesian inference is to generate enough samples from a random walk which adapts to the true posterior distribution  $P(\theta|D)$ . A variety of appropriate Markov chains can be constructed, but all of them are special cases of the Metropolis algorithm [8]. A study conducted by Kuczera and Parent (1998) demonstrated the capability of the Metropolis algorithm to produce reliable inferences for the parameter's uncertainty assessment in the case of hydrological models.

This posterior distribution represents the uncertainty in the model's parameters and can be propagated through a Monte Carlo method to assess the uncertainty in the model's output attributable to the parameters' uncertainties. However, as the obvious objective of calibration is to reduce the uncertainty in the model's output, it seems necessary to conduct global sensitivity analysis to determine on one hand, which parameters contribute the most to the output variation and require reducing their variances to minimize the variance in the model's output; and on the other hand, which parameters are insignificant and can be discarded from the model. Thus, using this method we can determine the type of research that is required to reduce the output's uncertainty by reducing the variance in some of the model's parameters.

There are many different ways to perform a sensitivity analysis, the method that will be used in this paper is called a "Variance based" method where the uncertainty in the model's output  $Y$  is measured by its variance  $V(Y)$  and thus can be partitioned to the sum of a top marginal variance and a bottom marginal variance as follows:

$$V(Y) = V[E(Y|U)] + E[V(Y|U)] \quad (2)$$

Where  $U$  is a subset of one or more elements  $\theta_i$ .  $V[E(Y|U)]$  is the variance of the conditional expectation of  $Y$  given  $U$  and it will be equal to zero if  $Y$  is completely independent of  $U$ ,  $E[V(Y|U)]$  is the expectation of the conditional variance of  $Y$  given  $U$  and it will be equal to zero if  $Y$  depends only on  $U$  [9]. In this context, the main effect, or first order sensitivity index  $S_U$ , representing the sensitivity of  $Y$  to the parameter  $U$  is defined as  $S_U = V[E(Y|U)]/V(Y)$ . The total effect, or total sensitivity index  $S_{TU}$  is defined as  $S_{Ti} = E[V(Y|\theta_{-U})]/V(Y)$  where  $\theta_{-U}$  indicates all the factors but  $U$ .

Many estimation procedures of  $S_U$  and  $S_{TU}$  are available in case of independent parameters. However, when the parameters are correlated, a replicated Latin Hypercube sampling method [9] for the estimation of the importance measure of parameters can be used.

## 4. MODEL ASSESSMENT METHOD

In this paper, a combination of two complementary and model – independent techniques is used to quantitatively assess the uncertainties associated with the model’s parameters as well as the output of the model itself.

### 4.1. Metropolis algorithm

Although the Metropolis algorithm is not the most efficient Markov Chain sampler, it is chosen in this study because of the simplicity of its implementation, and its generality. It only requires knowledge about the likelihood function to update simultaneously the parameters set for each iteration. Supposing that residuals between model and observation are  $N(0, \sigma^2)$ , the likelihood function can be written in the multiplicative form:

$$P(D | \theta) = \prod_{t=1}^n \frac{1}{(2 \cdot \pi \cdot \sigma^2)^{1/2}} \cdot e^{-\frac{(Y_t - f(X_t, \theta))^2}{2 \cdot \sigma^2}} \quad (3)$$

Where  $(Y_1, \dots, Y_n)$  is the vector of the measured response  $Y$ ,  $(X_1, \dots, X_n)$  is a vector of input data,  $\theta = (\theta_1, \dots, \theta_p)$  is the vector of  $p$  unknown parameters, and  $f(\cdot)$  is the model’s output.  $\sigma$  is considered, as well as  $\theta$ , as a set of parameters to be estimated during calibration.

At each iteration, candidate values of parameters are drawn from a multi-normal transition probability distribution for which the variance could be tuned up in a way to increase the speed of convergence. However, updating periodically (automatically) the variance during the simulation, as proposed by Kuczera [5] is subject to difficulties: how can one be sure that the samples used to update the variance contain information of a good quality that can help to ensure the convergence of the chain to the limit distribution? We suggest fixing a prior value of the variance according to the information about the parameters during all the simulation.

An interesting feature of the Metropolis algorithm is that the interaction among the model’s parameters is reflected in the likelihood function, so there will be no need to incorporate correlation in the prior distributions of parameters. In order to avoid favoring any initial value, the use of a uniform prior distribution over the range of parameters may seem reasonable [6].

### 4.2. Replicated Latin Hypercube sampling

The Replicated Latin Hypercube Sampling method r-LHS has been employed in this study to assess the importance measure of the parameters. This method use  $r$  replicate Latin hypercube samples of size  $k$  to produce  $m = r \times k$  parameter vectors  $\theta$  in total. The same  $k$  values of each component  $U$  of  $\theta$  will appear in each replicate but the matching within each one will be done independently. For this application the  $k$  values of each parameter  $U$  are sampled from its posterior distribution inferred with the Metropolis algorithm. The Iman & Conover rank correlation method [10] has been considered for the r-LHS in order to induce parameters’ correlation in the sample. After making the computer runs using the  $m$  replicated samples, the importance of  $U$  is assessed by computing the ratio  $S_U$ :

$$S_U = \frac{SSB}{SST}, \quad SSB = r \sum_{i=1}^k (\bar{y}_i - \bar{y})^2, \quad SST = \sum_{i=1}^k \sum_{j=1}^r (\bar{y}_{ij} - \bar{y})^2, \quad \bar{y}_i = \frac{1}{r} \sum_{j=1}^r y_{ij}, \quad \bar{y} = \frac{1}{k} \sum_{i=1}^k \bar{y}_i \quad (4)$$

$y_{ij}$  represents the output value that corresponds to the  $i$ th value  $U_i$ , in the  $j$ th replicate. In this paper, we are interested in the sensitivity analysis for the likelihood measure in order to identify the parameters that are mainly driving the model to have a good conformity with the data. Ratto [11] showed that sensitivity analysis for the likelihood gives useful information for model calibration especially when great interaction exists between parameters.

## 5. CASE STUDY

In this paper, we apply the method on the case of urban runoff modeling firstly on the scale of a sub-catchment as used in practice and secondly on the scale of a street surface.

### 5.1. Site description

Two different watershed scales have been used in this study: the first one WS1 is a 42 ha urban catchment (91% imperviousness) drained by a combined sewer system and the second one WS2 is a 160 m<sup>2</sup> street surface. The used rain event database covers a continuous period of 16 months (1996-1997) with 151 rain events. Suspended solid SS pollutographs\* were measured for 40 rain events at the outlet of the combined sewer, and for 11 rain events at a street gully collecting discharge from the street. These data were acquired on the experimental catchment “le Marais” in the centre of Paris [2].

### 5.2. Model description

The model used in this study to simulate the Suspended Solids pollutograph is a very classical one. It describes the particulate pollutants’ erosion during the storm event and their accumulation on the watershed during the preceding dry weather period. This model was at first proposed to be used on street surface scales. However, it is currently used in all available urban stormwater pollution software at the scale of urban subcatchment where both sewers and urban surfaces are described as one entity.

Equation 5 and Equation 6 represent the two accumulation models tested in this paper. Equation 5 calculates the accumulation of pollutants assumed to follow an asymptotic behavior that depends on two parameters: an accumulation rate  $Daccu$  (kg/ha/day) and a dry erosion rate  $Dero$  (day<sup>-1</sup>) [12].

$$\frac{dMa(t)}{dt} = Daccu \cdot Simp - Dero \cdot Ma(t) \quad (5)$$

$$\frac{dMa(t)}{dt} = Kaccu \cdot (M_{lim} \cdot Simp - Ma(t)) \quad (6)$$

Where  $Ma(t)$  (kg) is the available pollutants’ mass at time  $t$  and  $S_{imp}$  (ha) is the impervious area. Equation 6 represents a mathematical reformulation of the previous model and was chosen in regard to the obtained results. This model depends on two parameters: an accumulation coefficient  $Kaccu$  and a maximum accumulated mass  $M_{lim}$ . It supposes that the accumulation is proportional to the mass still to be accumulated before reaching the maximum  $M_{lim}$ , which is equivalent to the  $Daccu/Dero$ .

Equation 7 represents the evolution of the available pollutant mass during storm weather period. It is supposed that the eroded mass is proportional to the available mass and to the

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\* Suspended Solid pollutograph represents the profile of SS  $C(t)$  concentration during time  $t$

rainfall intensity. The erosion model depends on two parameters: the erosion coefficient  $Wero$  and a coefficient  $w$  [13].

$$C(t) = \frac{1}{q(t)} \cdot \frac{dMa(t)}{dt} \text{ and } \frac{dMa(t)}{dt} = -Wero \cdot I(t)^w \cdot Ma(t) \quad (7)$$

Where  $C(t)$  (mg/l) is the SS concentration produced by erosion,  $q(t)$  is the discharge (m<sup>3</sup>/s) at the outlet of the watershed at time  $t$ , and  $I(t)$  is the rainfall intensity (mm/hr).

### 5.3. Results

12,000 iterations were performed with the Metropolis algorithm, and the first 2,000 samples generated were removed allowing the Chain to “forget” the initial parameter set. Results showed that the Chain converged successfully to the same posterior probability distribution of the parameters regardless of the initial parameter set used. However, the speed of convergence has been found to be sensitive to the variance of the transition distribution. In the present case we chose a value of the standard deviation equal to 1/15 of the prior value of parameter to ensure the convergence.

#### 5.3.1. Marais catchment scale

Figure 2 represents the confidence intervals of the model’s output obtained by applying Monte Carlo to the model with the estimated posterior distribution of parameters. In the present case, the range of the possible responses is very large. The value of the estimated variance of errors ( $\sigma = 130\text{mg/l}$ ), which is quite large compared to the variance of the data ( $\sigma_{\text{data}} = 150 \text{ mg/l}$ ), indicates that the variation in the measured pollutographs are considered as randomness in regard to the predictive capacity of this calibrated model. Obviously, the proposed model seems to be unable to reproduce accurately the measured pollutographs, and the Metropolis results indicate clearly that it is not due to calibration problems.

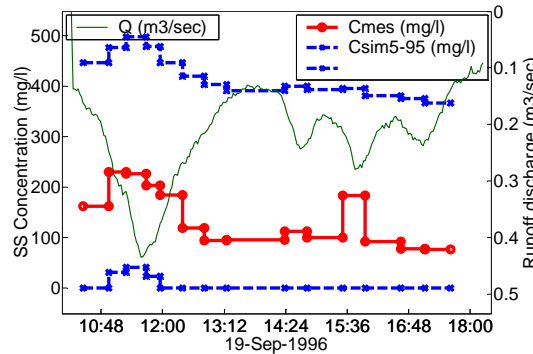


Figure 2 5-95% prediction intervals of the SS concentration at the Marais catchment scale

This is not surprising regarding the experimental results showed by Gromaire [2] where the deposits in combined sewer systems contribute to 60% of pollution. The complexity of sediments’ deposition, erosion and transport processes in sewers make the sub-catchment scale by far outside the domain of validity of the conceptual model used. Thus, it seems important to apply the MCMC method for the calibration of this model on a space scale having an acceptable range of conformity to the model’s domain of validity.

#### 5.3.2. Street Surface scale

Figure 3 presents the posterior probability distribution obtained for the parameters  $Daccu$ ,  $Dero$ ,  $Wero$ ,  $w$  and for the standard deviation of errors  $\sigma$  with the Metropolis algorithm.

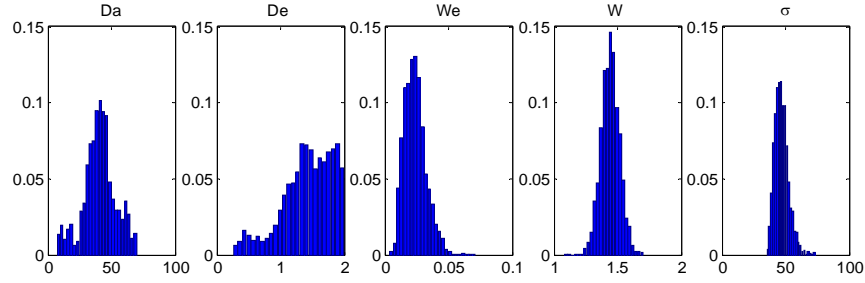


Figure 3 Posterior distribution of the 4 parameters estimated at the street catchment using Eq. 5

The analysis of the posterior distributions of the parameters shows large uncertainties related to the dry weather model parameters *Daccu* and *Dero* (Figure 4). We also found a linear correlation between these two parameters (correlation = 0.7). This correlation is due to the mathematical formulation of the accumulation model (Eq. 5). As a consequence, the accumulation model could be better calibrated if mathematically reformulated.

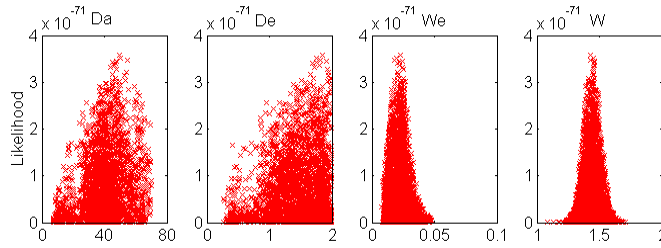


Figure 4 Scatter plot of the Likelihood measure vs. the parameters at the street catchment using Eq. 5

However, despite that the results obtained for the reformulated model (using Eq. 6) show a better identification of the maximum mass accumulated *Mlim* as shown in Figure 5, calibration results indicate a large uncertainty related to the parameter *Kaccu* representing (like the parameter *Dero*) the speed of the accumulation process during dry weather.

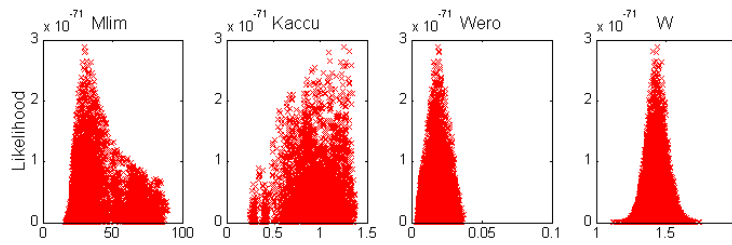


Figure 5 Scatter plot of the Likelihood measure vs. the parameters at the street catchment using Eq. 6

50 replicates of the 200 LH samples are used to estimate the importance measures of the parameters for the likelihood of the model's output for the two used models (Figure 6). Results show that the maximum accumulated mass *Mlim* represents an important parameter that has a significant impact on the likelihood measure of the model. However, the *Kaccu* parameter has an insignificant effect on the model's output. This conclusion is also provided using the scatter plot of the likelihood measure vs. the parameters as shown in Figure 4 & 5.

One can conclude that the estimation of the initial accumulated stock available before the rain event is very essential for the good performance of the model. However, the sensitivity analysis results indicate clearly that using the length of the dry weather period as an explicative parameter for the accumulation process, described by an asymptotic behavior, is not sufficient to explain the variability of the available mass just before the rain event.



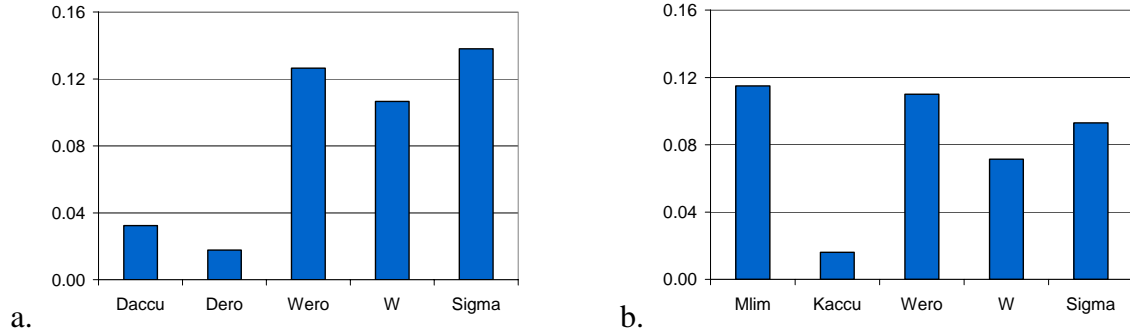


Figure 6 Importance measures for the likelihood measure of the model output using a. Eq 5 & b. Eq 6

Nevertheless, calibration results indicate a clear correlation between the maximum mass  $Mlim$  and the erosion parameter  $Wero$  (Figure 7.a.). Such correlation is not surprising regarding the mathematical structure of the erosion model (Eq. 7), which represents a multiplicative form of  $Ma(t)$  and  $Wero$ .

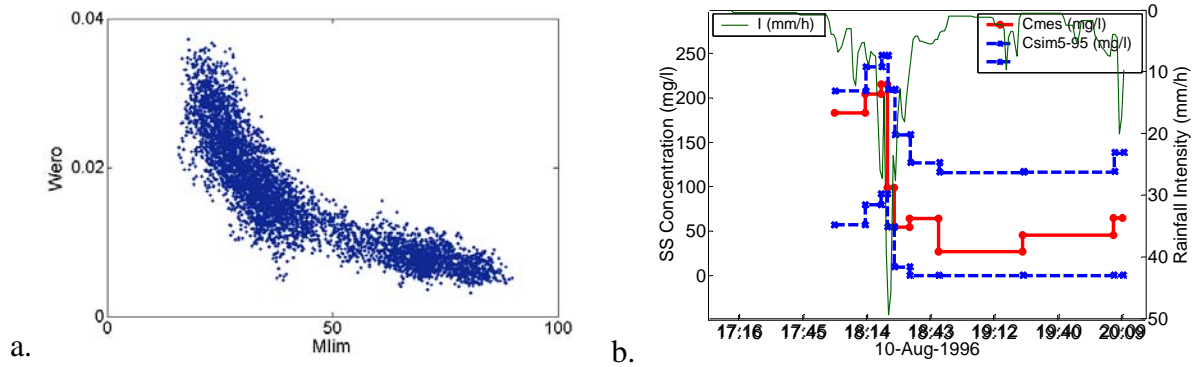


Figure 7 a. Correlations between  $Mlim$  and  $Wero$ . b. 5-95% prediction intervals of the pollutants concentration simulated by model

Figure 7.b. presents the confidence interval of the model's output  $C(t)$ . It shows large uncertainties in the model's predictions. This is not surprising regarding the fact that an important part of this uncertainty is attributable to the value of the variance of errors ( $\sigma = 47\text{mg/l}$ ) which is quite large compared to the variance of the data ( $\sigma_{\text{data}} = 62\text{mg/l}$ ). In other words, the predictive power of the calibrated model is low.

## 6. CONCLUSION

In this paper, we tested the applicability and effectiveness of a method used for model calibration/validation/sensitivity analysis in urban runoff quality modeling. This method, based on the MCMC sampling technique, consists of a combination of the Metropolis algorithm and a Variance based method. Metropolis algorithm provides an estimation of the posterior distributions describing parameters' uncertainties, as well as, their interaction structure. On the basis of the parameters' distributions, the Monte Carlo method determines the conceptual model's confidence intervals reflecting its prediction capacity. Using the posterior distribution, the performance of the replicated LHS method in regard to the likelihood measure leads to the quantitative identification of the main parameters that drive the model to have best fit to data.

Calibration results demonstrate that the tested conceptual model seems unable to represent the complexity of the system at the scale of urban sub-catchments. However, the application of the method to calibrate the model on a street surface scale shows that the mathematical concept of the accumulation model, using two parameters *Daccu* and *Dero*, contains linear interaction between its parameters, and implies much more uncertainty in their calibration. Furthermore, despite that a reformulation of this model using two parameters (*Mlim* and *Kaccu*) allows a better identification of the parameter *Mlim*, sensitivity analysis results show that the parameter *Kaccu* provides negligible contribution to the likelihood variation, or in other words, have no significant effect on the behavior of the model. This hypothesis casts doubts on the utility of using an asymptotic behavior, which depends only on the length of the dry weather period to describe the accumulation process. Such a conclusion needs to be validated on other sites to test its generality.

However, this method delivers much information, which would have been unreachable with classical calibration methods, and which are very useful for modeling attempts.

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