

A new empirical model for stormwater TSS event mean concentrations (EMCs)

Un nouveau modèle empirique de concentrations moyennes événementielles (CME) des matières en suspension des rejets urbains de temps de pluie

A. Dembélé^{1,2*}, J.-L. Bertrand-Krajewski¹, C. Becouze¹,
B. Barillon²

¹ Université de Lyon, INSA de Lyon, LGCIE, 34 avenue des Arts, F-69621
Villeurbanne cedex, France

² CIRSEE, Suez-Environnement, 38 rue du Président Wilson, F-78230 Le Pecq,
France

* E-mail : abel.dembele@insa-lyon.fr

ABSTRACT

An empirical model for TSS event mean concentrations in storm weather discharges has been derived from the analysis of data sets collected in two experimental catchments (Chassieu, separate system and Ecully, combined system) in Lyon, France. Preliminary tests have shown that the values of TSS EMCs were linked to the variable $X = TP \times ADWP$ (TP rainfall depth, $ADWP$ antecedent dry weather period) with two distinct behaviours under and above a threshold value of X named λ : EMCs are increasing if $X < \lambda$ and are decreasing if $X > \lambda$. An empirical equation is proposed for both behaviours. A specific calibration method is used to calibrate λ while the 4 other parameters of the model are calibrated by means of the Levenberg-Marquardt algorithm. The calibration results obtained with 8 events in both sites indicate that the model calibration is satisfactory: Nash Sutcliffe coefficients are all above 0.7. Monte Carlo simulations indicate a low variability of the model parameters for both sites. The model verification with 5 events in Chassieu shows maximum levels of uncertainty of approximately 20 %, equivalent to levels of uncertainty observed in the calibration phase.

KEYWORDS

Model, suspended solids, parameters, calibration, event mean concentrations, separate sewer system, combined sewer system.

RÉSUMÉ

L'analyse des données de deux sites expérimentaux (Chassieu, réseau séparatif pluvial et Ecully, réseau unitaire) à Lyon, France a permis d'obtenir un modèle empirique de concentrations moyennes événementielles des matières en suspensions des rejets urbains de temps de pluie. Les résultats préliminaires montrent que ces concentrations sont liées à la variable $X = TP \times ADWP$ (TP hauteur précipitée, $ADWP$ période de temps sec antérieure) et qu'elles présentent deux comportements différents autour d'une valeur seuil λ : elles augmentent tant que $X < \lambda$ et diminuent lorsque $X > \lambda$. Une équation empirique de ces deux comportements a été proposée. Un algorithme spécifique a été développé pour l'estimation du paramètre λ et les 4 autres paramètres ont été estimés en appliquant l'algorithme de Levenberg-Marquardt. Pour chaque site, le modèle a été calé avec les données de 8 événements pluvieux. Les résultats du calage du modèle pour chaque site sont satisfaisants car tous les coefficients de Nash Sutcliffe obtenus sont supérieurs à 0.7. Les résultats obtenus par simulations de Monte Carlo montrent une variabilité faible des estimations des paramètres du modèle pour les deux sites. La vérification du modèle a été effectuée avec les données de 5 événements du site de Chassieu et l'incertitude maximale observée est équivalente à celle de calage, soit 20 % environ.

MOTS CLÉS

Modèle, matières en suspension, paramètres, calage, concentrations moyennes événementielles, réseau séparatif pluvial, réseau unitaire.

1 INTRODUCTION

Since three decades, urban stormwater quality models (USQMs), with various levels of complexity and objectives, have mostly been developed and applied by researchers (Gromaire *et al.* 2002). Recently, because of increasing regulatory constraints, in particular the European Water Framework Directive - WFD (EC, 2000), operators of urban water systems have shown more interest in knowledge about and possible applications of USQMs.

From an operational point of view, the estimation of event pollutant concentrations and loads is frequently the first objective, in particular for TSS (total suspended solids) which are the vector of many other pollutants observed to a large extent in the particulate phase. This estimation can be based on measurement campaigns, with sampling and laboratory analyses. However, practical and financial limitations do not allow monitoring all events. Continuous *in situ* monitoring could be a valuable alternative, but it is still not well developed by practitioners. Consequently, USQMs, if appropriately calibrated and tested, represent another way to estimate concentrations and loads. Among all USQMs, event mean concentrations (EMC) models appear as an acceptable compromise between over-simplified site mean concentration models and multi-processes complex models, with some capacity to account for the inter-event variability of EMCs (Mourad, 2005).

The most frequent type of EMC models are multi-regression models. Their calibration is strongly sensitive to available experimental data (Mourad *et al.*, 2005; Dembélé *et al.*, 2009). Moreover, regression models usually do not have a structure or even variables which explain, at least globally, the build-up and washoff processes which have been recognised as two of the most influencing processes determining pollutant concentrations and loads. Explanatory variables in regression models are selected in the most cases according to both their availability and some numerical criteria (coefficient of correlation or variance analysis for example).

A new empirical EMC model has been developed because existing regression models appear very poor to reproduce observed data for two experimental catchments. This model is also an attempt to introduce some explanatory aspects in the empirical equations. The paper presents the methodology to derive the model structure, the calibration procedure and the main first results obtained for two catchments in Lyon, France: Chassieu (separate sewer system) and Ecully (combined sewer system).

2 EXPÉRIMENTAL SITES AND DATA SETS

The data used have been collected in two experimental sites with different characteristics, land-use and sewer systems: their main characteristics are given in Table 1. The active area is the catchment area which contributes effectively to the runoff. It is estimated as the product of the total catchment area by the mean runoff coefficient which is itself calculated as the ratio runoff volume / rainfall volume. Both sites, which are part of the OTHU project (Field Observatory on Urban Hydrology, www.othu.org), are equipped with sensors measuring quantitative (flow depth and flow velocity) and qualitative (turbidity, conductivity, pH and temperature) parameters.

Site characteristics	Ecully	Chassieu
Location	West of Lyon	East of Lyon
Land use	Residential	Industrial
Total area (ha)	245	185
Active area (ha)	60	54
Mean slope (%)	2	0.4
Percent of impervious area (%)	42	75
Sewer system	Combined	Separated

Table 1. Main characteristics of Chassieu and Ecully experimental sites

The part of the dataset used for this study (see Table 2) contains TSS EMCs and rainfall characteristics (antecedent dry weather period *ADWP* and rainfall depth *TP*). The TSS EMC is measured after 0.45 μm filtration of the event mean sample collected by means of a Bülher 4010 auto-sampler. The TSS analysis is carried out according to the French standard NF EN 872. The raw rainfall data recorded by an OTT Pluvio 200 weighing rain gauge are processed automatically to calculate the rainfall characteristics (Dembélé, 2008).

3 METHODOLOGY

This section describes the data analysis, the mathematical formulation of the model, the calibration method and the uncertainty evaluation.

3.1 Data analysis

Some key values (coefficient of variation CV, minimum, mean and maximum values) of the variables used in this study are given in Table 2. For both sites, inter-event variability is very significant, as indicated by coefficients of variation. For example, CVs of the rainfall depths in Chassieu and Ecully are respectively equal to 125 % and 139 %. Orders of magnitude are equivalent for both sites. For example, the coefficients of variations of TSS EMCs are equal to 63 %. However, TSS EMCs in Ecully are globally higher than in Chassieu, which is explained by the significant contribution of wastewater in the combined system in Ecully.

	Chassieu (13 events)				Ecully (8 events)			
	Min	Mean	Max	CV (%)	Min	Mean	Max	CV (%)
TSS EMCs (mg/L)	24	90	230	63	57	140	284	63
Rainfall depth TP (mm)	0.68	10.27	38.17	125	2.02	8.74	37.41	139
$ADWP$ (days)	0.35	1.53	4.52	82	0.20	1.13	4.69	118

Table 2. Data and statistics [$ADWP$ = antecedent dry weather period]

Various regression models have been tested in order to estimate TSS EMCs without positive results (results not detailed here). After several attempts to identify key variables, an alternative approach has been applied to the data set. The first hypothesis consists to assume that the pollutant build-up and washoff processes, which should explain to some extent the EMC values, can be approximated and considered as mainly related respectively to the antecedent dry weather $ADWP$ and to the rainfall depth TP . As in many other approaches (e.g. Freni *et al.*, 2009, Soonthornnonda *et al.*, 2008), this assumption considers that the pollutant mass available on the catchment surface for a given storm event is linked to the $ADWP$: the longer the $ADWP$, the larger the accumulated pollutant mass. Similarly, it is assumed that the washoff process at event scale is mainly related to the rainfall depth: the pollutant mass transferred to the sewer system is increasing with rainfall depth, provided a sufficient mass of pollutant has been accumulated before the event.

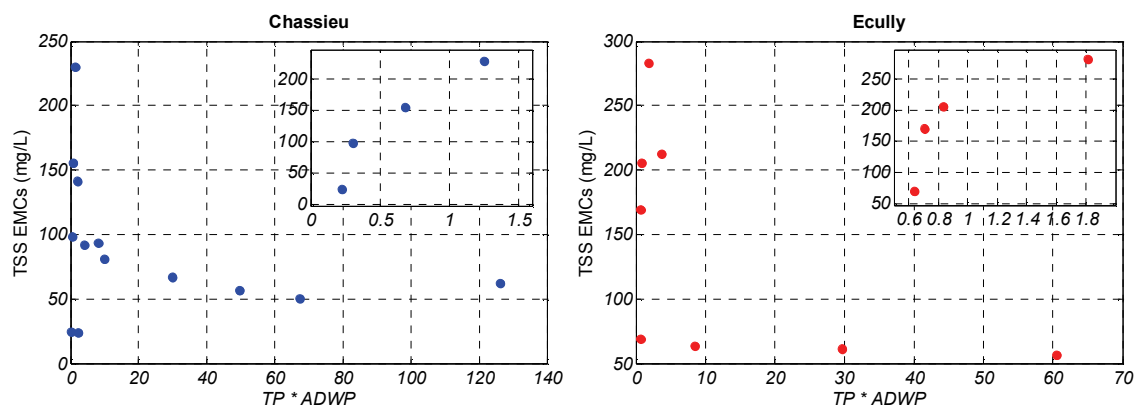


Figure 1. Relationship between TSS EMCs and the variable $TP \times ADWP$ in Chassieu (left) and Ecully (right), with a zoom for the region of low values of $TP \times ADWP$

Based on the above hypotheses, the relationship between EMC values and the product $TP \times ADWP$ has been explored. The results for both catchments are shown in Figure 1. This relationship appears clearly non-monotonic. For both sites, TSS EMCs increase until a threshold value of $TP \times ADWP$ named λ and then decrease when $TP \times ADWP$ increases more. We assume that these two parts correspond to two distinct behaviours. In the first rising part, the EMC increases with the rainfall depth which is the limiting factor. In the second declining part, the EMC decreases with the rainfall depth as the accumulated mass is the limiting factor: when rainfall depth increases for a given mass, there is a dilution effect and EMC decreases. Similar observations have been described by other authors, e.g.

Sheng *et al.* (2008).

3.2 Equations of the model

Based on the above graphs, and noting X the product $TP \times ADWP$, one may conclude that i) the TSS EMC increases while X is lower or equal to λ and ii) it decreases when X is greater than λ . Looking at the graphs, the following equation has been proposed after tests of various possibilities:

$$\frac{dEMC}{dX} = \frac{b_1}{X}(X \leq \lambda) + \frac{-b_3}{X^2}(X > \lambda) \quad \text{Eq. 1}$$

with EMC the TSS EMC (mg/L), $X = TP \times ADWP$ with TP in mm and $ADWP$ in days, λ the threshold value of X separating the two behaviours of EMC values, b_1 and b_2 model parameters.

The final equation of the model is obtained by analytical integration of Eq. 1 :

$$EMC = [(b_1 \ln(X) + b_2)(X \leq \lambda)] + \left[\left(\frac{b_3}{X} + b_4 \right) (X > \lambda) \right] \quad \text{Eq. 2}$$

with b_1 , b_2 , b_3 and b_4 the model parameters.

The first part of the model assumes a logarithmic increase of TSS EMCs while $X \leq \lambda$. The second part assumes that the decrease of TSS EMCs is proportional to $1/X$ for $X > \lambda$.

3.3 Model calibration

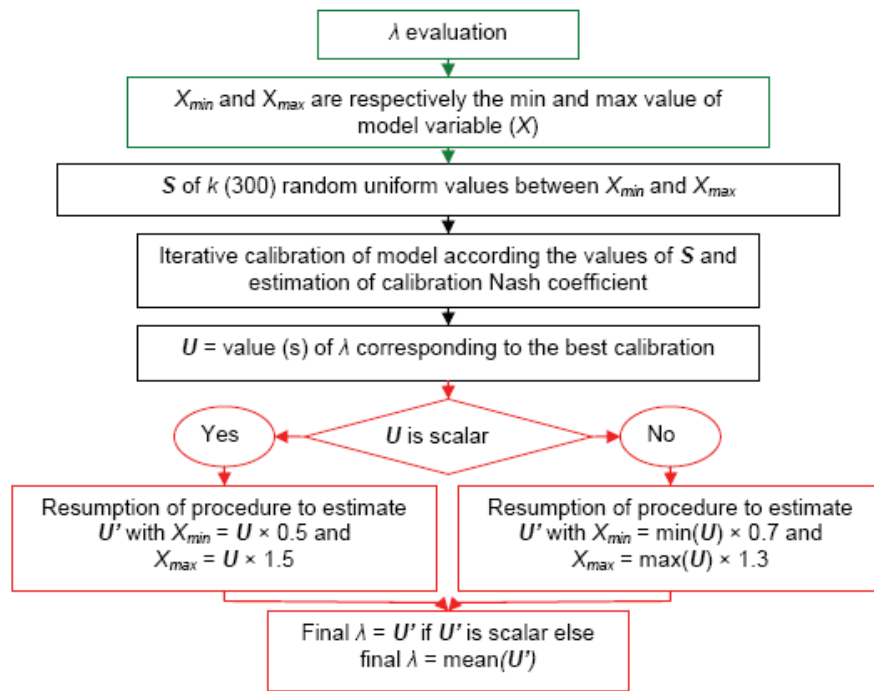
The model calibration is carried out in two steps, due to the nature of the five parameters. The Levenberg-Marquardt algorithm (LMA) (More, 1977) is used to estimate b_1 , b_2 , b_3 and b_4 . A specific algorithm has been developed to estimate λ . Indeed, λ is a threshold criteria applied to the values of X , hence its first derivative does not exist, which is not compatible with the LMA.

The parameter λ must be calibrated first, with the algorithm schematized on Figure 2. A vector \mathbf{S} is generated, with $k = 300$ random values uniformly sampled between the minimal and maximal observed values of X , noted X_{min} and X_{max} . Each element of \mathbf{S} is considered iteratively as a possible value of λ . The model is calibrated by using the Nash Sutcliffe coefficient (Nash and Sutcliffe, 1970) (Eq. 3). At the end of the k iterations, two situations are possible. In the first one, one and only one value of $\lambda = \mathbf{U}$ gives the best calibration, i.e. the highest value of the Nash coefficient. In the second one, several values of λ stored in the vector \mathbf{U} may give the same best calibration: it is not possible to determine a unique best value of λ at this stage. In both cases, the procedure is repeated with new values of X_{min} and X_{max} : $X_{min} = \mathbf{U} \times 0.5$ and $X_{max} = \mathbf{U} \times 1.5$ in the first case; $X_{min} = \min(\mathbf{U}) \times 0.7$ and $X_{max} = \max(\mathbf{U}) \times 1.3$ in the second case. The resulting new value is \mathbf{U}' . In the last step, if \mathbf{U}' is a scalar, the final value of λ is taken equal to \mathbf{U}' , else it is taken equal to the mean value of the vector \mathbf{U}' .

$$Nash = 1 - \frac{\sum_{i=1}^n (EMC_{Sim} - EMC_{obs})^2}{\sum_{i=1}^n (EMC_{obs} - \overline{EMC_{obs}})^2} \quad \text{Eq. 3}$$

with EMC_{sim} = estimated TSS EMCs, EMC_{obs} = measured TSS EMCs which mean value is $\overline{EMC_{obs}}$ and n = number of events.

The LMA is one of the most useful numerical optimization methods due to its robustness. In theory, it provides a numerical solution to the problem of minimizing a function (generally nonlinear) over a set of parameters \mathbf{p} . The LMA interpolates between the Gauss-Newton algorithm (GNA) and the method of gradient descent. It is an iterative procedure which provides a vector of parameters \mathbf{p} corresponding to the minimal value (at least in theory) of an objective function in the least squares sense (Eq. 4). In most cases, the LMA provides a solution even if starting with initial \mathbf{p} far off the final minimum, classically $\mathbf{p}^T = (1, 1 \dots 1)$.

Figure 2. Algorithm for the calibration of λ

$$fob(p) = \sum_{j=1}^m [y_i - f(x_i|p)]^2 \quad \text{Eq. 4}$$

with fob the objective function, y_i the i^{th} observation of the variable to be modelled, f the analytical function of the model, x_i the i^{th} observation of the explanatory variable, p the vector containing the model parameters and m the number of observations.

3.4 Evaluation of uncertainties

Uncertainties of model estimations are evaluated by means of Monte-Carlo simulations. This method consists to associate to each input variable of the model a probability of distribution of frequency (PDF). The choice of this associated distribution (e.g., uniform, normal, lognormal) is crucial to avoid biased estimations. This choice must take into account all available information about the input variables (i.e. analytical method, sampling protocol). N independent random samples are created for each input variable according to its PDF. The model is calibrated with every sample. The N values obtained for each parameter allows determining their empirical distributions. Uncertainties of the model estimations are evaluated according to these empirical distributions.

4 RESULTS AND DISCUSSION

For each site, the model has been calibrated with 8 events. For Chassieu, the 8 first events are used in chronological order of measurement. The 5 remaining events are used for model verification. For Ecully, all 8 events have been used for calibration.

Monte Carlo simulations have been carried out with $N = 3000$ runs. As an initial hypothesis, PDFs are normal distributions with a standard deviation of 20 % of the mean value. Two calibrations have been compared: i) direct calibration DC with measured values of all variables without accounting for uncertainties, ii) Monte Carlo calibration MC.

Table 3 gives the estimated values of the model parameters. Figure 3 and Figure 4 show the histograms of the model parameters. For both sites, parameter values obtained with DC are very close to mean values obtained with MC. The coefficients of variation of the parameters for MC are relatively low (maximum 47 %), which means that the model calibration is rather stable, as shown in Figure 3 and Figure 4. However, CVs may significantly differ between sites. For example, CV of λ is equal to

8 % in Chassieu and 17 % in Ecully.

Nash Sutcliffe coefficients are all above 0.7. The Nash Sutcliffe coefficients with DC are equal to 0.78 in Chassieu and 0.91 in Ecully. The mean values of the Nash Sutcliffe coefficients with MC are equal to 0.78 in Chassieu (with CV = 5 %) and 0.90 in Ecully (with CV = 2 %). In comparison (detailed data not presented here), Nash Sutcliffe coefficients obtained for other tested traditional regression models (e.g. Mourad, 2005) are negative, as sometimes reported by other authors, e.g. Dotto *et al.* (2009).

Parameters and Nash coefficients	Chassieu			Ecully		
	DC	MC (3000 runs)		DC	MC (3000 runs)	
		M	CV (%)		M	CV (%)
b_1	111.44	107.28	15	483.68	524.50	47
b_2	204.62	201.38	5	305.02	321.80	29
b_3	63.92	67.12	49	458.34	462	5
b_4	63.83	53.21	5	44.96	44.60	5
λ	1.62	1.63	8	1.5	1.4	16.69
Nash coeff.	0.78	0.78	5	0.91	0.90	2

Table 3. Parameters and Nash Sutcliffe coefficients for calibration (DC = calibration with measured values and MC = calibration with Monte-Carlo samples).

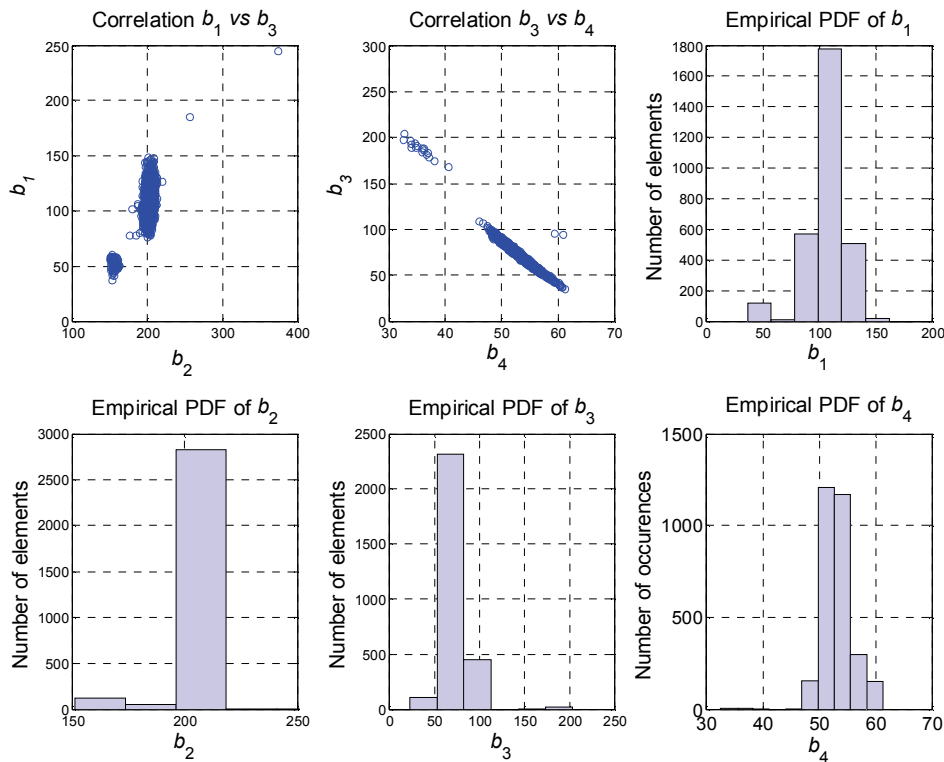


Figure 3. Correlation analysis and empirical PDFs of the model parameters in Chassieu

Correlation analysis between b_1 and b_2 on one hand and b_3 and b_4 on the other hand (Figure 3 and Figure 4) indicate that these correlations are significant, particularly between b_1 and b_2 in Ecully. If this trend is confirmed with further tests in progress, the model will be reformulated to account for this correlation. Figure 5 shows the histograms of the threshold parameter λ and the Nash coefficients for Chassieu (left) and Ecully (right). As with the other parameters b_1 , b_2 , b_3 and b_4 , the variability is rather low. For example, 95 % of the Nash coefficient values are in the range [0.67 - 0.83] in Chassieu and in the range [0.86 - 0.94] in Ecully. Empirical distributions of the model parameters appear skewed and non-normal. But, according to the central limit theorem with large samples, the mean values can nevertheless be considered as the best estimations. Further Monte Carlo simulations are in progress in order to further analyse these trends with more data sets and more catchments.

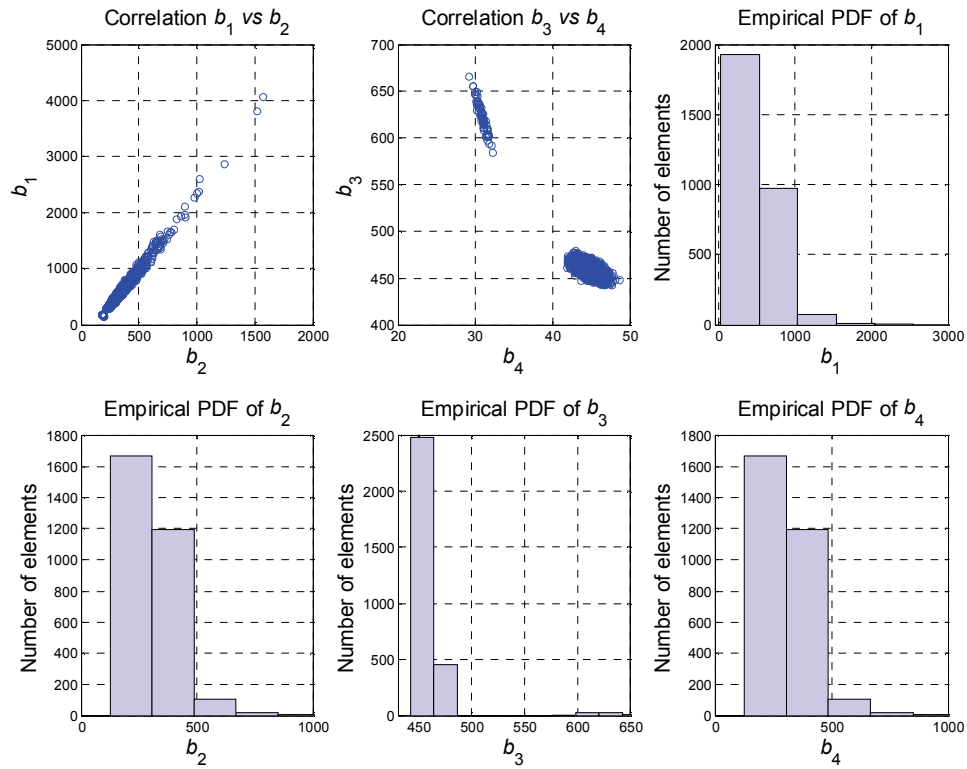


Figure 4. Correlation analysis and empirical PDFs of the model parameters in Ecully

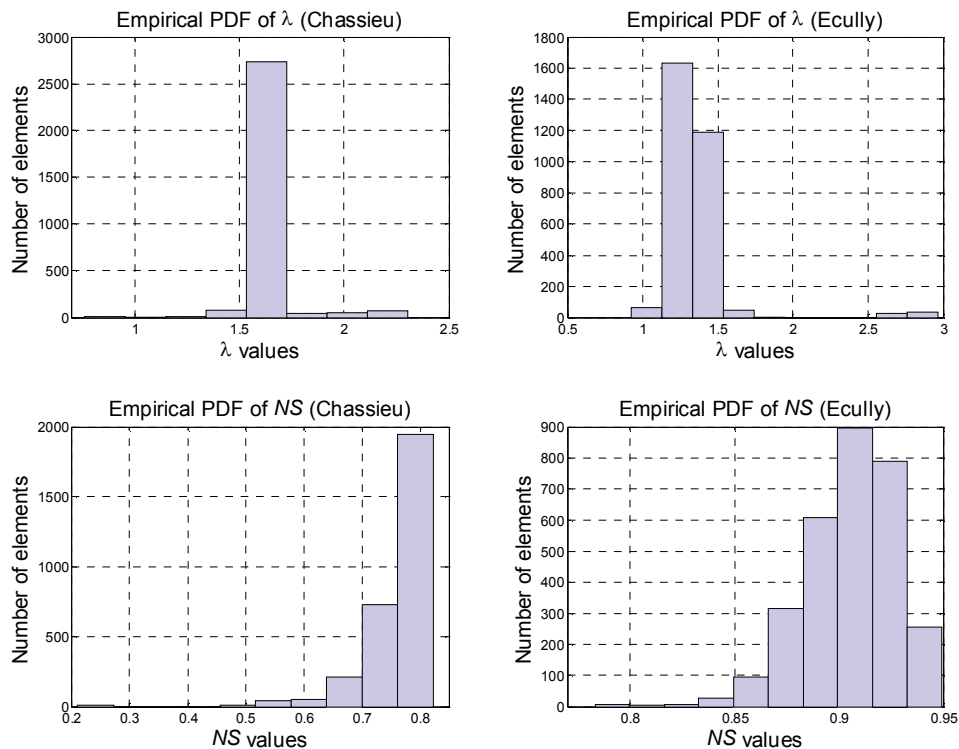


Figure 5. Empirical PDFs of the parameter λ and calibration Nash-Sutcliffe coefficients (NS)

Figure 6 shows the comparison between measured and simulated values of TSS EMCs with 95 % confidence intervals. For both sites, the mean values of calibration uncertainties are less than 20 %. Low TSS EMCs show the largest uncertainty. The prediction uncertainty of the 5 test events in

Chassieu (green circles in Figure 6), not used in calibration, is likewise less than 20 %. These uncertainties are rather equal to the calibration uncertainties, which indicate that, with this limited data set, the model can be as satisfactory for Chassieu.

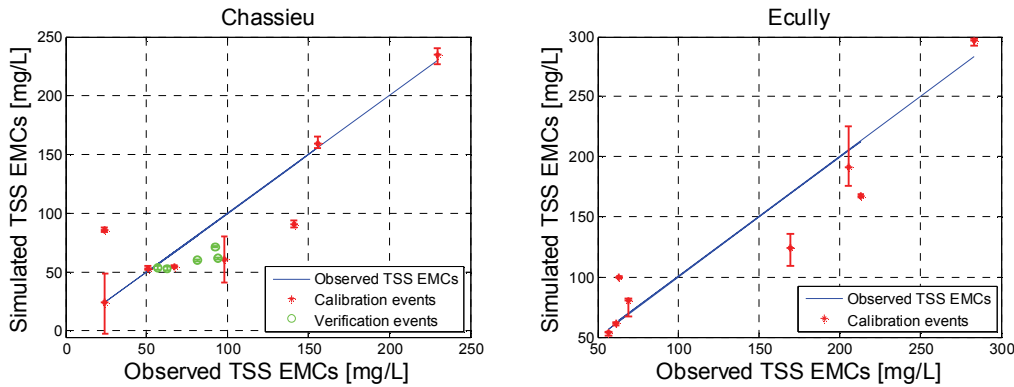


Figure 6. Comparison between measured and simulated TSS EMCs

Other results have been obtained for the 42 ha combined catchment Le Marais in Paris, France with 64 storm events (Chebbo and Gromaire, 2004). Data analyses show that the rising part of Eq. 2 is not necessary in this case: the second term where TSS EMCs decrease when X increases is sufficient to describe the observed TSS EMCs. In this case, the accumulated mass of pollutants would not be the limiting factor and the rainfall depth appears as the main factor influencing TSS EMCs. Therefore, the model formulation was adapted (Eq. 5) to the data of this catchment and $ADWP$ was replaced by the rainfall duration Rd in the expression of in X . Eq. 5 and its integral form Eq. 6 mean that the TSS EMCs decreases when the rainfall volume increases. Results with Eq. 6 using $N = 3000$ Monte-Carlo simulations are summarised in Figure 7. Graph 1 shows the empirical PDF of the parameter C . Graph 2 shows the model calibration results and graph 3 the empirical PDF of the calibration Nash-Sutcliffe coefficients (NS). Dashed isolines on each side of the bisector solid line in graph 3 represent respectively the $\pm 10, 25, 50, 75$ and 90% values of the observations and the circle areas are inversely proportional to the uncertainties of the estimated values. The mean values of calibration uncertainties are less than 20% (graph 2) and all the calibration NS values are positive with a mean value equals to 0.5 (graph 3). Thus, model calibration can be considered as satisfactory. The calibrated model has been verified by the Leave-one-out cross validation (LOOCV) method (Rudemo, 1982). In LOOCV, one single observation from the data set is kept for verification and all other observations are used for calibration data. This is repeated in such a way that each observation is used once for verification. LOOCV results are shown in graph 4. As for calibration, the mean values of calibration uncertainties are less than 20% . Moreover, the mean value of the verification NS value is also approximately equal to 0.5 . These results are compatible with the hypothesis that significant amounts of easily mobile dry weather deposits are present in this catchment and contribute significantly to wet weather TSS loads (Chebbo and Gromaire, 2004).

$$\frac{dEMC_M}{dX} = \frac{-C}{X^2} \quad \text{Eq. 5}$$

$$EMC_M = C \times \left(\frac{1}{X} + 1 \right) \quad \text{Eq. 6}$$

with $X = Rd \times TP$ with Rd the rainfall duration (hours).

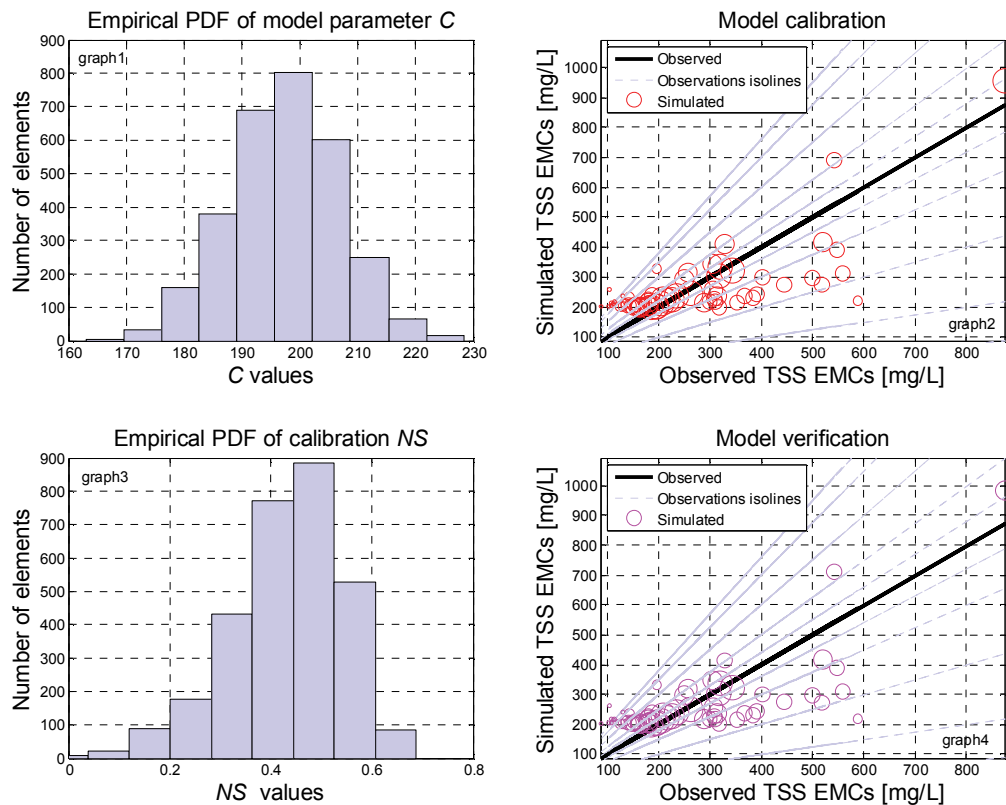


Figure 7. Results of the Le Marais catchment with 64 storm events

These results show that the proposed empirical TSS EMCs model performs well in case of the Chassieu and Ecully catchments. The model calibration with 8 events for both sites gives satisfactory results (Nash-Sutcliffe coefficients higher than 0.7). The performance of the model verification with 5 events in Chassieu is equivalent to the calibration performance. In addition, the results obtained in case of the Le Marais catchment show that the model can be easily reformulated according to the outcomes of a preliminary data analysis. In this second model formulation, only one parameter is necessary.

Compared to detailed dynamic pollutant models (e. g. Freni *et al.*, 2009; Chen and Adams, 2006), this simple model aims to estimate only EMCs and not the detailed variations of the concentration with time and it comprises a much less number of parameters. Moreover, the model requires only simple informations (rainfall depth, rainfall duration and antecedent dry weather period) and it can be easily adapted to new data sets.

5 CONCLUSIONS

An empirical model for TSS event mean concentrations in storm weather discharges has been derived from the analysis of data sets collected in two experimental catchments (Chassieu, separate system and Ecully, combined system) in Lyon, France. Preliminary tests have shown that the values of TSS EMCs were linked to the variable $X = TP \times ADWP$ with two distinct behaviours under and above a threshold value of X named λ : EMCs are increasing if $X < \lambda$ and are decreasing if $X > \lambda$. An empirical equation is proposed for both behaviours. A specific calibration method is used to calibrate λ while the 4 other parameters of the model are calibrated by means of the Levenberg-Marquardt algorithm.

The calibration results obtained with 8 events in both sites indicate that the model calibration is satisfactory: Nash Sutcliffe coefficients are all above 0.7. Monte Carlo simulations indicate a low variability of the model parameters for both sites. The model verification with 5 events in Chassieu shows maximum levels of uncertainty of approximately 20 %, equivalent to levels of uncertainty observed in the calibration phase.

The second model version adapted to and tested with 64 events measured in the Le Marais catchment

shows that Nash Sutcliffe coefficients of approximately 0.5, which can be considered as satisfactory for such a simple model formulation with a unique parameter.

Based on the above first results, further model tests are in progress for TSS EMCs with more than 200 events measured in the Chassieu and Ecully sites. Tests will also be carried out for other pollutants EMCs, especially metallic and organic priority pollutants.

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