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## **TSS, COD and priority pollutants in stormwater – Event fluxes modelling using conceptual approach**

MES, DCO et polluants prioritaires des rejets urbains de  
temps de pluie - Modélisation des flux événementiels par  
approche conceptuelle

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### **RÉSUMÉ**

Les versions originales et modifiées d'un modèle conceptuel ont été évaluées pour la prédiction des flux (M/ha) événementiels des polluants des rejets urbains de temps de pluie. Les polluants concernés incluent les matières en suspension MES, la demande chimique en oxygène DCO et des polluants prioritaires de la directive cadre européenne sur l'eau (WFD, 2000/60/CE). Les deux versions du modèle se composent chacun de deux modules : i) un module d'accumulation des polluants en temps sec à la surface du bassin versant et un module de transport des polluants en temps de pluie. Les deux versions ont en commun le même module de transport mais diffèrent par leurs modules de d'accumulation : de type exponentiel et donc asymptotique pour la version originale et logarithmique pour la version modifiée. Les résultats montrent que les deux versions du modèle sont valables pour la prédiction des flux événementiels par temps de pluie de la plupart des polluants étudiés et que les performances obtenues dépendent aussi bien du polluant que des caractéristiques du site étudié. Toutefois, avec seulement deux paramètres à estimer (optimiser) contre quatre, la version modifiée du modèle donne des performances globalement meilleures que celles obtenues avec la version originale.

### **ABSTRACT**

The original and modified versions of a conceptual model have been evaluated for predicting the stormwater pollutant event fluxes (M/ha). studied pollutants include the total suspended solids TSS, the chemical oxygen demand COD and the European Water Framework Directive (WFD, 2000/60/CE) priority pollutants. Both versions of the model contain two modules: i) the buildup module which allows estimating the pollutant mass accumulated on the catchment surface during the dry period preceding a rainfall event and ii) the washoff module which is used to estimate the pollutant events masses contained in the runoff volume. Both versions of the model contain the same washoff module and differ by the buildup module: exponential asymptotic for the original version and logarithmic for the modified version. The results show that both the two evaluated versions of the model have the satisfying performances and that the level of these performances depends to the pollutant type and the concerned catchment characteristics. However, having only two parameters to be estimated against four, the performances of the modified model are globally higher than these of the original model.

### **KEYWORDS**

Buildup, Calibration, COD, Conceptual model, Priority pollutants, TSS, Verification, Washoff

## 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 fluxes is frequently the first objective, in particular for TSS (total suspended solids) which are the vector of many other pollutants, including priority 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 urban stormwater pollutant fluxes. Among all USQMs, event fluxes (EF) models appear as an acceptable compromise between over-simplified site mean fluxes models and multi-processes complex models, with some capacity to account for the inter-event variability of EFs (Mourad, 2005).

The most frequent type of EFs 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 fluxes. 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).

The original and modified versions of the classical and very popular conceptual model (Chen and Adams, 2006) are been evaluated with the datasets from two catchments in France. The development of a modified version of this model aims to ameliorate the predictive capability of the original version. The paper presents the description of both versions of the model, the calibration and verification procedures and the main results obtained for two catchments in Lyon, France: Chassieu (separate sewer system) and Ecully (combined sewer system).

## 2 EXPERIMENTAL 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 summarised 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](http://www.othu.org)), are equipped with sensors measuring quantitative (flow depth and flow velocity) and qualitative (turbidity, conductivity, pH and temperature) parameters.

Table 1. Main characteristics of Chassieu and Ecully experimental sites

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

The part of the dataset used for this study (see **Table 3**) contains on the one hand TSS, COD and some priority pollutants EMCs and the other hand rainfall characteristics (antecedent dry weather period ADWP and rainfall depth TP). Event mean samples, used for measure the pollutants EMCs, were collected by means of a Bülher 4010 auto-sampler. The TSS EMC is measured after 0.45 µm filtration of the event mean sample and its analysis is carried out according to the French standard NF EN 872. The analysis methods of COD and priority pollutants are summarised **Table 2**. The particulate fraction is considered as a residue after 0.45 µm filtration where the dissolved fraction is a filtrate. The raw rainfall data recorded by an OTT Pluvio 200 weighing rain gauge are processed automatically to calculate the rainfall characteristics (Dembélé, 2008).

Table 2. Pollutants and analysis methods

Pollutants	Analysis methods	Standard reference
TSS	Filtration after 0.45 µm	NF EN 872
Particulate and dissolved COD	Micro-method of Dr. Lange	AFNOR T.90-101
Particulate and dissolved fractions of priority metals	ICP-MS (inductively Coupled Plasma Mass Spectrometry)	NF EN ISO 7294-1/2
Particulate and dissolved fractions of priority organic pollutants	Multi-residue method using GC-MS (Gas Chromatography – Mass Spectrometry ) and LC-FLD-MS/MS (Liquid Chromatography Fluorescence Detection Mass Spectroscopy/Mass Spectroscopy)	/

### 3 METHODOLOGY

This section describes the calculation technique of pollutant event fluxes, used models, calibration and verification methods used.

#### 3.1 Estimation of pollutant event fluxes

Pollutant event flux  $EF$  is considered in this study as the product of its  $EMC$  and mass, divided by the active area of the catchment for a given rainfall event.  $EF$  is calculated by (1).

$$EF_p = \frac{EMC_p \times V_e}{A_a} \quad (1)$$

with  $EF_{obs}$  is the observed pollutant  $p$  event flux (M/ha active),  $EMC$  the pollutant  $p$  event mean concentration (µg/l),  $V_e$  the runoff volume (m<sup>3</sup>) of rainfall event  $e$  and  $A_a$  the active area (ha).

#### 3.2 Model description

As mentioned above, two different model formulations are used in this study: the classical formulation of the conceptual pollutant buildup – washoff model and a modified version including a new formulation of the pollutant buildup module.

##### 3.2.1 The original version of classically conceptual model

It is the very popular conceptual model used in many stormwater pollutant (TSS principally) modelling problems (e.g. Shaheen, 1975; Alley and Smith, 1981; Delectic et al. 1997; Chen and Adams, 2006). This model contains two modules: i) the pollutant buildup module (2) and ii) the pollutant washoff module (4). As is shown in equation (3), the final formulation of the equation (2) after analytical integration, the amount of pollutant to be accumulated on the catchment surface during antecedent dry period have an asymptotic value. This formulation is based on an assumption on which, the dispersion due to both the wind and the sweeping streets avoid the amount of pollutant accumulation rise continually. This may be a disadvantage of the formulation of model due to fact it will probably underrate systematically the pollutant fluxes higher than the values of fluxes used in the calibration

process.

$$\frac{dM}{dADWP} = b_0 + b_1 M \quad (2)$$

$$M = \frac{b_0}{b_1} (1 - e^{-b_1 ADWP}) + M_0 e^{-b_1 ADWP} \quad (3)$$

$$EF = M (1 - e^{-b_2 TP}) \quad (4)$$

with  $M$  (kg/ha) the amount of pollutant per unit area on the catchment surface after a rainfall,  $b_0$  (kg/ha×h) is a constant rate of the pollutant deposition,  $b_1$  (h<sup>-1</sup>) constant pollutant removal rate, ADWP a antecedent dry period (h), and  $TP$  (m<sup>3</sup>) a runoff event volume.

### 3.2.2 The modified version of model

In tentative to deal the underrating problem mentioned above, we propose in equation (5) a new formulation of the buildup module, the washoff module being conserved. As showed in equation (6), the final formulation of equation (5) after analytical integration, this new logarithmic formulation of the pollutant buildup is not asymptotic and contains only one parameter  $C$ . Theoretically, our new formulation of the pollutant buildup module includes two information: i) the pollutant mass accumulated rise with the antecedent dry period duration and ii) but the growth rate decreases with the antecedent dry period duration.

$$\frac{dM}{dADWP} = \frac{1}{ADWP} \quad (5)$$

$$M = \ln(ADWP) + C \quad (6)$$

with  $C$  is a constant.

### 3.3 Model calibration and verification methods

The Levenberg-Marquardt algorithm (LMA) (More, 1977) is used to estimate  $b_0$ ,  $b_1$ ,  $b_2$ ,  $M_0$ , and  $C$  (see equations from (2) to (6)). 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 by minimizing a function (generally nonlinear) over a set of parameters  $p$ . 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  $p$  corresponding to the minimal value (at least in theory) of an objective function in the least squares sense (7). In most cases, the LMA provides a solution even if starting with initial  $p$  far off the final minimum, classically  $p^T = (1, 1, \dots, 1)$ .

$$fob(p) = \sum_{j=1}^m [y_i - f(x_i | p)]^2 \quad (7)$$

with  $fob$  the objective function,  $y_i$  the  $i^{th}$  observation of the variable to be modelled,  $f$  the analytical function of the mode (equations (3) and (4) for the original model and equations (4) and (6) for modified model),  $x_i$  the  $i^{th}$  observation of the explanatory variable,  $p$  the vector containing the model parameters and  $m$  the number of observations.

The verification consists to the evaluation of the predictive capability of calibrated model. The verification method used in this study is 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.

Both calibration and verification performance is evaluated according the calculated value of The Nash-Sutcliffe coefficient (Nash and Sutcliffe, 1970; Legates and McCabe, 1999) (8). This coefficient is one of the most used in hydrology (e.g. Sauquet and Leblois, 2001; Gopakumar et al., 2007; McIntyre and Al-Qurashi, 2009). It can take values from minus infinite (bad performance) to 1 (perfect performance). In practice, positive value of *NS* coefficient can be considered as satisfying performance.

$$NS = \frac{\sum_{k=1}^N (S_k - O_k)^2}{\sum_{k=1}^N (O_k - \bar{O})^2} \quad (8)$$

with *NS* is the Nash-Sutcliffe coefficient value [·], *S<sub>k</sub>* and *O<sub>k</sub>* respectively the observed and calculated using model of a *k<sup>th</sup>* value of the variable, *N* is a number of observations and  $\bar{O}$  a mean value of the observed values of the variable.

## 4 RESULTS AND DISCUSSION

The main results of this study are summarised **Table 3**. Mean LOOCV value indicates the mean value of different calibrations of the model using the LOOCV method. In each square bracket, the value in left concerns the original version of model where the value on right concerns the modified version.

According to these results, both original and modified version of the model can be considered as useful to predict on both the classical stormwater pollutant (TSS and COD) and most of the priority pollutants event fluxes. Model performances vary with the pollutant and the catchment characteristics (combined and separate sewer systems). Globally, the performance of both original and modified version seems to be higher for TSS and COD than for the priority pollutants (see **Figure 1** for TSS in Chassieu and **Figure 2** for Simazine in Ecully). This can be explained partly by the random nature of priority pollutants: the variance of priority pollutant EMCs in different runoff volume is very high. Indeed, whatever a rainfall event, a corresponding runoff contains systematically a quantifiable concentration of TSS and COD. That is not a case for priority pollutants. For example for a comparable rainfall event in term of runoff volume, the great difference of a quantity of a given priority is that any logical explanation can be give. This is especially true for non metal priority pollutants as Simazine and Atrazine which use is otherwise banned in France since about ten years ago. Concerning the difference between both experimental sites, the performance of the model seems to be globally higher in Chassieu than Ecully. This difference can be explained by the difference of sewer system. Indeed, Ecully being equipped to the combined sewer system and it clear that the runoff volume collected here is a mixing of runoff from rainfall and wastewater. This latter factor is not explicitly taking account in the model formulations.

As comparison between both original and modified versions of model, it seems globally that the predictive performance of modified version is on average higher than that of the original version. It is a case for example for TSS in Chassieu (see **Table 3** and **Figure 1**). In the **Figure 1**, graphs 1, 2 and 3 are obtained using the original version of model and graphs 4, 5 and 6 are obtained using the modified version of model. The graphs 1 and 4 show the results of calibration using full dataset. More the estimated values of TSS (red-asterisk) is close to the corresponding observation (black line), more the performance of calibration is high. It can be concluded that the performance of calibration of both versions of model is high and similar: *NS* = 0.90. The graphs 2 and 5 show the different values of the Nash-Sutcliffe coefficients obtained in the calibration process using the Leave-one out cross validation method. These values, all higher than 0.8, confirm the very good performance of calibration of both version of the model. The graphs 3 and 6 show the results of model verification. If the performance of the verification of both versions of the model is very satisfying, it appears clearly that of modified version (graph 6) with *NS* = 0.88 is higher than that of the original version (graph 3) with *NS* = 0.80. This difference seems to be linked to underrating, using the original version of the model, of the predictive value of the high observe value of TSS as mentioned in the paragraph 3.

Another example of graphical results is showed **Figure 2**. It is the results for Simazine in Ecully catchment. Both calibration and verification performances of both versions of model can be considered as quasi similar and satisfying.

Table 3. Summary of the modelling results: the Nash-Sutcliffe coefficient values of calibration and verification

Catchments	Pollutants	Estimated values of Nash-Sutcliffe coefficient					
		Calibration				Verification [Original    Modified]	
		Full data [Original    Modified]		Mean LOOCV [Original    Modified]			
Chassieu	TSS	[0.90	0.90]	[0.90	0.90]	[0.80	0.88]
	Total COD	[0.74	0.72]	[0.74	0.68]	[0.30	0.66]
	Particulate Pb	[0.98	0.87]	[0.98	0.87]	[0.92	0.75]
	Total Pb	[0.95	0.83]	[0.98	0.87]	[0.93	0.76]
	Atrazine	[0.95	0.83]	[0.94	0.85]	[0.44	-0.13]
	Diuron	[0.86	0.85]	[0.87	0.85]	[0.70	0.75]
	Fluoranthene	[0.92	0.85]	[0.90	0.40]	[-0.62	0.83]
	Simazine	[0.95	0.74]	[0.91	0.75]	[0.37	-0.14]
Ecully	TSS	[0.58	0.55]	[0.58	0.55]	[0.37	0.35]
	Total COD	[0.45	0.55]	[0.67	0.56]	[0.08	0.29]
	Particulate Pb	[0.80	0.60]	[0.78	0.62]	[0.17	-1.07]
	Total Pb	[0.82	0.64]	[0.82	0.70]	[0.36	-0.70]
	Atrazine	[0.71	0.65]	[0.78	0.65]	[-0.60	-0.30]
	Diuron	[0.84	0.89]	[0.85	0.70]	[0.33	0.35]
	Particulate Fluoranthene	[0.36	-0.27]	[0.43	-0.31]	[-0.74	-1.07]
	Simazine	[0.88	0.81]	[0.91	0.81]	[0.69	0.67]

## 5 CONCLUSIONS

The datasets from two different catchments in France, Chassieu equipped with the separated sewer system and Ecully equipped with a combined sewer system, are been use to evaluate the predictive performance of two different stormwater quality models. It is the original version and a new modified version of the classical popular conceptual model. Evaluated pollutants include TSS, COD and priority pollutants. Both versions contain two modules: i) the buildup module which allows estimating the pollutant mass accumulated on the catchment surface during the dry period preceding a rainfall event and ii) the washoff module which is used to estimate the pollutant mass contained in the runoff volume. The two versions of model contain the same washoff module and differ by the buildup module: exponential asymptotic for the original version and logarithmic for the modified version. The original model contains 4 parameters to be estimated (optimised) against 2 for the modified version.

The results show that both the two evaluated versions of the model have the satisfactory performance and the level of these performances depends to the pollutant type and the catchment characteristics. However, in comparison term, the performances of the modified model, in spite of the lower number of parameters, are globally higher than these of the original model.

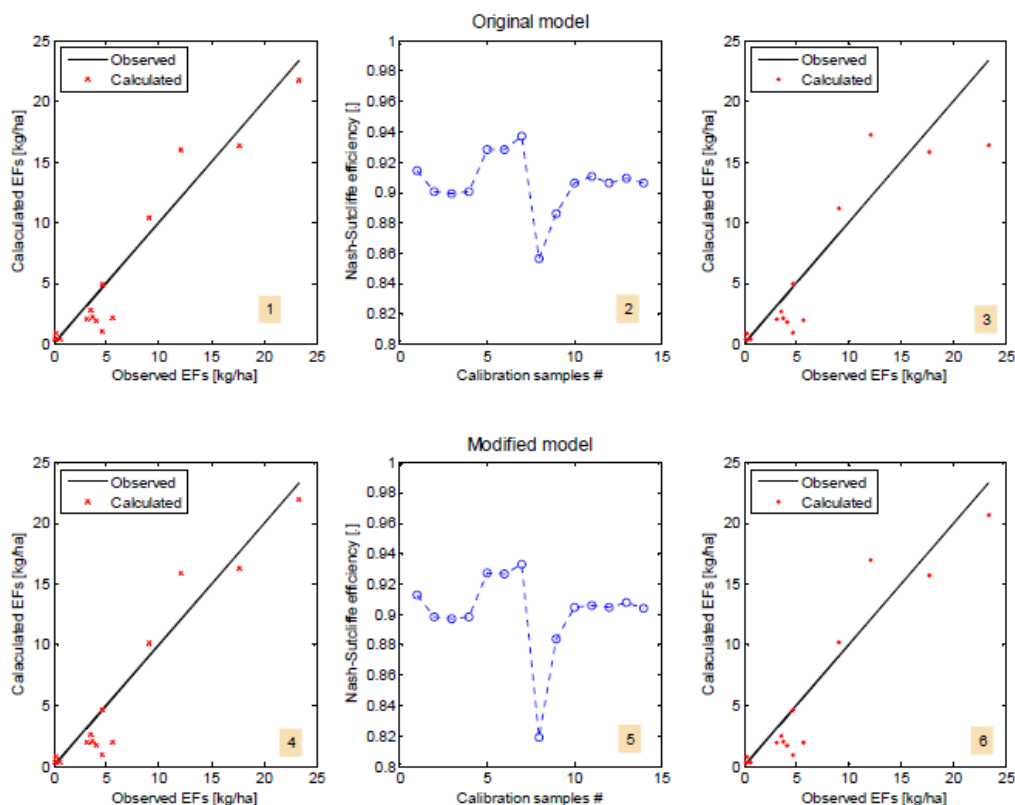


Figure 1. Results from original (at the top) and modified (at the bottom) models for TSS for Chassieu catchment

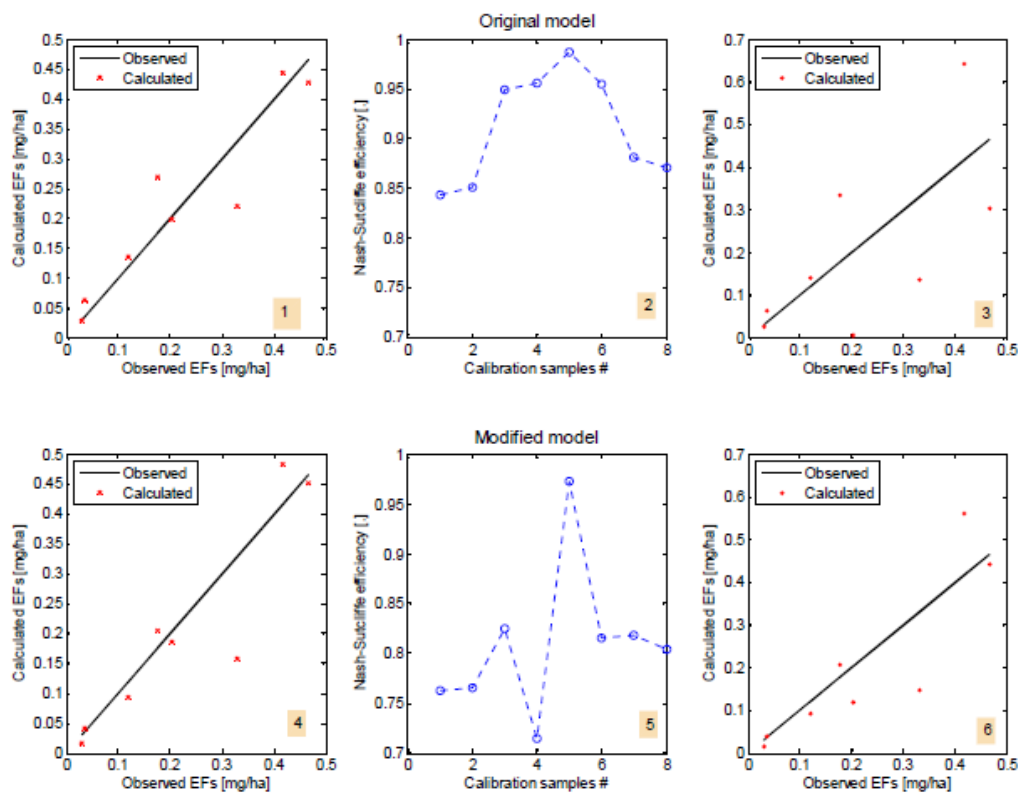


Figure 2. Results from original (at the top) and modified (at the bottom) models for Simazine for Ecully catchment



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