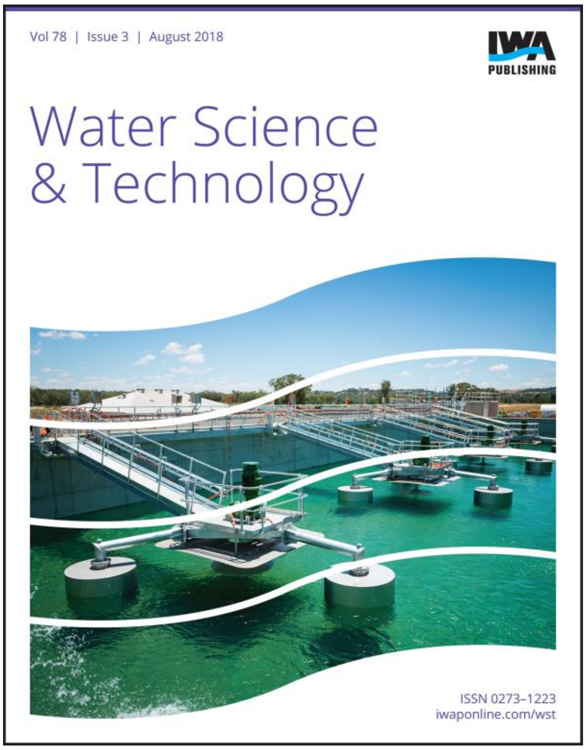
Vol 78 | Issue 3 | August 2018
IWA PUBLISHING
Water Science & Technology
ISSN 0273-1223
iwaponline.com/wst

Revisiting conceptual stormwater quality models by reconstructing virtual state variables

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ABSTRACT

This work proposes a Bayesian non-informative reconstruction of virtual state variables in the representation of stormwater total suspended solids pollutographs by the traditional wash-off models, based on 255 rainfall events measured in a 185 ha French urban catchment. Results from event-based analyses revealed the missing representation of an essential process in the traditional rating curve (RC) model (simplest wash-off model) for 56% of the rainfall events. The unsatisfactory performances of the RC model are found to be not necessarily linked to antecedent dry weather conditions, as assumed by a great number of accumulation/wash-off models. Statistical tests suggest that non-representable rainfall events by the RC model are randomly distributed in time. The proposed Bayesian reconstructions of a potential process missed by the RC model exhibit a suitable identifiability at an intra-event scale. However, these reconstructions are not interpretable from the traditional accumulation/wash-off notions, i.e. in terms of a unique state of virtual available mass over the catchment that is decreasing over time, due to their high unrepeatability regarding their shape and their low prediction capacity for other rainfall events.

Key words | conceptual modelling, error models, existence and unicity of solutions, functional data clustering, identifiability, time-variable parameters

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INTRODUCTION

During the past 40 years, modelling the dynamics of stormwater total suspended solids (TSS) loads at the outlet of urban catchments has been mainly addressed by the idea of accumulation/wash-off (originally by Sartor *et al.* (1974)). Although this conceptual model does not constitute a rigorous physical description of the system, it is usually considered as a physically based model in the sense that it is based on mass conservation principles and its parameters can be interpretable from a physical point of view (Bonhomme & Petrucci 2017). Indeed, this accumulation/wash-off model has been implemented in a massive amount of literature and a wide variety of urban catchments (size, land use, complexity), for purposes such as real time control, climate change assessment, risk analysis, water management, and in multiple commercial software tools. However, the unsatisfactory performance of this approach is frequently reported, as well as the difficulty of generalizing its results to real world applications, especially as urban catchments are large and complex (e.g. Vaze & Chiew 2003; Deletic *et al.* 2012).

The accumulation/wash-off original model relies on the idea of a virtual 'mean' state of TSS mass over the catchment that is accumulated during dry periods and is later on washed off by rainfall and runoff, producing the TSS load at the outlet of the catchment. However, this notion from Sartor *et al.* (1974), followed by various analogue formulations (e.g. Egodawatta *et al.* 2009; Freni *et al.* 2009; Crobedu & Bennis 2011) has been developed under the following experimental/methodological settings: (i) controlled experimental conditions in small scale systems, (ii) limited number of TSS data, (iii) limited number of rainfall events, and (v) limited assessment of uncertainty in data and model parameters. This suggests how uncertainty linked to application of these models outside their limits (e.g. in large and complex urban catchments – see Liu *et al.* (2012)) is expected to be amplified.

Furthermore, the existence of a 'mean' state of available TSS mass for large catchments (from 100–200 ha) has been questioned from a low identifiability and a high spatial variability of model parameters (Bonhomme & Petrucci 2017).

doi: 10.2166/wst.2018.337

This hypothesis can be nourished from satisfactory results when applying a simplified rating curve (RC) model (Huber *et al.* 1988) without including a 'mean' available mass term (e.g. Kanso *et al.* 2005). Under this perspective, one can ask for the existence of a deterministic global process missed by the RC model, essential to represent the pollutant loads, which is oversimplified or misinterpreted by the accumulation/wash-off idea.

For this purpose, the time variable parameters (TVPs) concept has been introduced in the hydrological and environmental context as a powerful statistical model-based approach to describe unobserved processes or state variables (e.g. Young 2013). The TVP method reconstructs the potential temporal dynamics of the optimal parameters for a given model. TVPs can be used with transfer function models estimated using instrumental variables (e.g. Young 2013), or with general conceptual models within Bayesian frameworks (Renard *et al.* 2010). Indeed, Bayesian total error analysis (BATEA) (Kuczera *et al.* 2006) has emerged as a promising model-based TVP estimation technique for reconstructing unmeasured inputs or state variables, adaptable to non-linear and complex model structures, including flexibility in the error model of the reconstructed state variable (e.g. for rainfall time series reconstruction – see Leonhardt *et al.* (2014)).

This paper aims to revisit the accumulation/wash-off idea by using Bayesian TVP reconstructions, scrutinizing for evidence of a deterministic global process and its interpretability as a 'mean' state of available pollutant mass being washed by rainfall. Furthermore, this accumulation/wash-off model structure is sought to be reformulated by analysing the inter-event repeatability of the reconstructed state variables. The experimental/methodological settings aimed at overcoming the limitations of previous studies by considering: (i) an urban catchment of 185 ha, (ii) TSS load measurements with a temporal resolution of 2 minutes (with data uncertainty), (iii) 255 rainfall events (from 2004 to 2011), (iv) the state-of-art calibration and parameter uncertainties assessment (Bayesian methods, e.g. Kuczera *et al.* (2006)).

MATERIALS AND METHODS

Accumulation/wash-off model

The original accumulation/wash-off model from Sartor *et al.* (1974) describes the stormwater TSS load (kg) at the outlet of an urban catchment as the product of two factors: a sediment mass $M(t)$ (kg) and a removal factor $W(t)$ (-). In this representation, $M(t)$ is a decaying state variable of a virtual available stock mass which in the end limits the load production given by a wash-off process $W(t)$. Sartor *et al.* (1974) describe the two terms as follows, including a set of calibration parameters:

$$load(t) = M(t) \cdot W(t) = M_0 \cdot e^{-a \cdot Q(t)^r \cdot t} \cdot a \cdot Q(t)^r \quad (1)$$

where M_0 (kg) is the initial condition from which M starts to decay ($M(0) = M_0$, with $t = 0$ the beginning of a rainfall event), and a and r express the influence of the stormwater flow $Q(t)$ (m^3/s) on the removed TSS mass. Several different formulations for M and W during rainfall events can be found in the literature and some examples are given in Table 1.

Among these formulations, the simplest one is called 'infinite stock' or RC (Huber *et al.* 1988), where M is considered constant ($M = M_0$) and the wash-off term shows a non-linear relation to the flow:

$$load(t) = M_0 \cdot Q(t)^r \quad (2)$$

In this case, the calibration parameters are reduced to two (M_0 and r).

As a generality, it can be seen that for most model structures $0 < M(t) \leq M_0$ and $dM/dt \leq 0$ for all t during rainfall

Table 1 | Examples of different wash-off formulations for the accumulation/wash-off model

Formulations			
M (kg)	**W (-)**	**Parameters**	**Reference**
$M_0 \cdot e^{-a \cdot Q(t)^r \cdot t}$	$a \cdot Q(t)^r$	M_0, a, r	Sartor *et al.* (1974)
$M_0 \cdot (1 - e^{-C1 \cdot Q(t)^{C1} \cdot t})$	$C1 \cdot Q(t)^{C2}$	$M_0, C1, C2$	Freni *et al.* (2009)
$M_0 \cdot C1 \cdot (1 - e^{-C2 \cdot Q(t) \cdot t})$	$C2 \cdot Q(t)$	$M_0, C1, C2$	Egodawatta *et al.* (2009)
1	$M_0 \cdot Q(t)^r$	M_0, r	Huber *et al.* (1988) (RC model)

events, M being described as either a time variable or a constant process (e.g. Table 1). Indeed, the RC model in Equation (2) can be directly linked with any time variable formulation of M (as in Equation (1)), by making M_0 a TVP. Therefore, this work proposes to undertake Bayesian reconstructions of the 'virtual' state variable M by adopting the RC traditional model in Equation (2) and replacing M_0 by a TVP, $\hat{M}(t)$, keeping r as a calibration parameter (formulation F1). The $\hat{M}(t)$ estimation in F1 can be directly compared to a time constant or variable traditional M formulation (e.g. Table 1). As a complementary analysis, a second formulation (F2) is explored, in which the RC model is modified with $\hat{r}(t)$ (-) as the TVP to be reconstructed and M_0 as a calibration parameter.

Experimental setup

The proposed methods are tested with information about 255 rainfall events from the Chassieu urban catchment (Lyon, France), measured between 2004 and 2011. This is one of the experimental sites of the OTHU project (Field Observatory for Urban Hydrology – www.othu.org). The basin is a 185 ha industrial area drained by a separate storm sewer system, with imperviousness and runoff coefficients of about 0.72 and 0.43 respectively. Flow rate Q (L/s) and TSS concentrations (mg/L) at the outlet of the catchment are measured in a 1.6 m circular concrete pipe with a 2 minute time-step resolution. Q is calculated from water depth with a relative standard uncertainty from 15% to 25%. Regarding TSS concentrations, the drainage water is pumped into an off-line monitoring flume in a shelter, where turbidity measurements (NTU) are converted into TSS concentration values by local calibration functions (see Sun et al. 2015). The standard uncertainties in the estimated TSS concentrations ranged from 11% to 30%. The uncertainties of the TSS load (kg) are propagated by the law of propagation of uncertainties (LPU) (ISO 2009), obtaining relative standard uncertainties from 15% to 50%. Standard uncertainties become higher for higher values of the measurands (Q, TSS concentration, $load$).

Bayesian reconstruction of virtual state variables by time variable parameters

The reconstruction of a virtual state variable by TVPs consists in solving a calibration problem where a TVP is represented as a time series of parameters rather than a singular time-constant parameter. In principle, every time-step of a TVP can be considered as an independent parameter in the inference scheme, with a length equal to the length of the output series load. However, the dimensionality of this problem will be massive, risking over-parametrization and delivering incorrect estimations (Vrugt et al. 2009). To avoid this over-parametrization in the inference, the TVP time series has usually a coarser temporal resolution than the output data. For this purpose, a time window strategy is adopted, reducing the dimensionality of the problem by dividing the TVP reconstruction into equally spaced time windows (see e.g. Sun & Bertrand-Krajewski 2013). For this case, a further test with non-equally spaced time windows based in the cumulative volume reported results analogous to the equally spaced time windows approach.

This TVP ($\hat{M}(t)$ for F1 or $\hat{r}(t)$ for F2) is proposed to be estimated jointly with the other set of regular calibration parameters θ by means of a Bayesian inference scheme. Therefore, the joint posterior probability density function (PDF) of θ and TVP are calculated by Equation (3) as $p(\theta, TVP/Q_{obs}(t), load_{obs}(t))$, given the input $Q_{obs}(t)$ and output $load_{obs}(t)$ data with some prior knowledge about θ and TVP (from BATEA in Kuczera et al. (2006)). The values of θ and TVP values with the maximum likelihood in the estimation of the joint posterior PDF $p(\theta, TVP/Q_{obs}(t), load_{obs}(t))$ are assumed be the 'optimal' parameters θ_{opt} and TVP_{opt} ($\hat{M}(t)_{opt}$ for F1 or $\hat{r}(t)_{opt}$ for F2).

$$p(\theta, \hat{M}(t)/Q_{obs}(t), load_{obs}(t)) \alpha \prod_{t=1}^{n} \frac{1}{\sqrt{2\pi\hat{\sigma}load_t^2}} exp\left[-\frac{1}{2}\frac{(load_{sim}(Q_{obs}(t), \theta, TVP) - load_{obs}(t))^2}{\hat{\sigma}load_t^2}\right] \cdot p(\theta) \cdot \prod_{t=1}^{n} \frac{1}{\sqrt{2\pi\hat{\sigma}TVP^2}} exp\left[-\frac{1}{2}\frac{Var(TVP)}{\hat{\sigma}TVP^2}\right] p(TVP) \quad (3)$$

where n is the total observed load values in $load_{obs}(t)$. The $load_{sim}(Q_{obs}(t), \theta, TVP)$ is the simulated load by the input flow rate series $Q_{obs}(t)$ and a set of θ and TVP. $p(\theta)$ and $p(TVP)$ represent a prior belief about the probability that a candidate set of θ and TVP values are 'true' (assumed as a non-informative uniform distribution for all cases). Equation (3) allows the explicit separation of the model error of TVP (second Pi product) from the error model of the output $load$ (first Pi product). With the purpose of finding a TVP estimation 'as constant as possible in time' (and therefore less informative), the error model of TVP (second Pi product) is assumed to be proportional to the TVP's own variance $Var(TVP)$. This constraint is aimed at avoiding 'curve fitting' the TVP with $load_{obs}(t)$.

Both error models, for the *load* and TVP estimations (first and second Pi product respectively), are assumed to be independent and normally distributed, with the error variances $\hat{\sigma}load_t^2$ and $\hat{\sigma}TVP^2$, respectively. $\hat{\sigma}load_t^2$ is considered heteroscedastic, being equal to the square of the standard uncertainty of each observed value $load_{obs}(t)$ (e.g. Sun & Bertrand-Krajewski 2013). On the other hand, $\hat{\sigma}TVP^2$ is considered to be homoscedastic and is estimated as another parameter in the set θ (e.g. Sage *et al.* 2015), expressed as $\hat{\sigma}M^2$ (kg) for F1 and $\hat{\sigma}r^2$ (-) for F2. The same Equation (3) is used for calibrating the RC model, by omitting the second Pi product term, delivering $p(\theta/Q, load)$ as a posterior probabilistic characterization of θ (with θ_{opt} also for the optimal parameters).

The DREAM algorithm (Vrugt 2016) is applied to solve Equation (3) and to evaluate the three formulations (the traditional RC, the F1 and F2 formulations) for the different θ and *TVP* variants (Table 2). The logarithmic form of Equation (3) is implemented to ensure numerical stability and a maximum number of simulations of 6×10^5 is used with a maximum of 30 parallel Markov Chains to reach convergence (Gelman and Rubin (GR) convergence criteria >1.2, see Gelman & Rubin (1992)). The TVP reconstructions are undertaken with a resolution of 12 time windows (i.e. equivalent to 12 parameters, see Table 2), balancing between the convergence of the algorithm (GR $>$ 1.2) and capturing the global dynamics of the TVPs (see application in Sun & Bertrand-Krajewski (2013)). Table 2 also summarizes the parameters' minimum and maximum values search ranges in the prior uniform distributions $p(\theta)$ and $p(TVP)$ in Equation (3). These ranges are defined for r and M_0 based on the literature (Kanso *et al.* 2005) and are equally adopted for each window of $\hat{M}(t)$ and $\hat{r}(t)$. The maximum of the error variances $\hat{\sigma}M^2$ and $\hat{\sigma}r^2$ are defined, respectively, as four times the standard deviation of M_0 and r in the RC calibration.

The parameters θ and the reconstruction of virtual state variables *TVP* are estimated for each individual rainfall event (event-based calibration). This eliminated the need for a 'dry build up' model (e.g. Freni *et al.* 2009) as the initial sediment mass (M_0) is directly estimated for each rainfall event.

For each *i*th calibration event, the results for the different formulations proposed in Table 2 (posterior probabilities and optimal parameter sets) provide the basis for revisiting some of the traditional accumulation wash-off ideas. This is performed by looking at:

(i) a relationship between the Nash–Sutcliffe efficiency (NS_i) (comparing $load_{sim}(t)_i$ and $load_{obs}(t)_i$) obtained from the RC model event-based calibration, as an evidence of a process potentially missed by this model structure, and the antecedent dry weather period of the rainfall event ($ADWP_i$). This linkage is evaluated by considering further characteristics of the rainfall events (mean and maximum flow rate and the date of the event) in addition to the ADWP, into a principal component analysis (PCA) (*relation of RC model performance to inter-event characteristics*).

(ii) the NS_i (comparing $load_{sim}(t)_i$ and $load_{obs}(t)_i$) for the event-based reconstructions TVP_i in the F1 and F2 formulations, besides the well-posedness and identifiability of the inferred joint posterior PDFs, $p(\theta, TVP/Q, load)_i$ (*intra-event identifiability of a potential process missed by RC model*).

(iii) similarities in the shape or dynamics of the $TVP_{opt\,i}$ estimation with other reconstructions, obtained from different rainfall events (*inter-event identifiability from repeatability*).

(iv) the capacity of a given set of $\theta_{opt\,i}$ and $TVP_{opt\,i}$ to represent the load in another rainfall event, evaluated by the NS (*inter-event transferability*, see Bardossy & Singh (2008)).

(v) further hypotheses about a potential missing process based on physical knowledge about the system and the obtained results (*interpretability*).

RESULTS AND DISCUSSION

The available data and simulation results from a local event-based calibration with the RC model and the F1 and F2 formulations applied to event $i = 16$ are shown as an example

Table 2 | DREAM solving of Equation (3) for virtual state variables reconstruction formulations, specifying the set of parameters θ and TVP, the total number of parameters and the minimum and maximum search range in the prior distributions p(θ) and p(TVP)

Formulation	Parameters θ	TVP	Number of parameters θ + TVP	Minimum/maximum search range values
RC model	r (-), M_0 (kg)	–	2	r (0, 5); M_0 (0, 8×10^5)
F1	r (-), $\hat{\sigma}M^2$ (kg)	$\hat{M}(t)$ (kg)	$2+12=14$	r (0, 5); $\hat{M}(t)$ (0, 8×10^5) for each t; $\hat{\sigma}M^2$ (0, 2.4×10^5)
F2	M_0 (kg), $\hat{\sigma}r^2$ (-)	$\hat{r}(t)$ (-)	$2+12=14$	M_0 (0, 8×10^5); $\hat{r}(t)$ (0, 5) for each t; $\hat{\sigma}r^2$ (0, 1.5)