Comparative uncertainty analysis of copper loads in stormwater systems using GLUE and grey-box modeling

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Abstract In this paper two attempts to assess the uncertainty involved with model predictions of copper loads from stormwater systems are made. In the first attempt, the GLUE methodology is applied to derive model parameter sets that result in model outputs encompassing a significant number of the measurements. In the second attempt the conceptual model is reformulated to a grey-box model followed by parameter estimation. Given data from an extensive measurement campaign, the two methods suggest that the output of the stormwater pollution model is associated with significant uncertainty. With the proposed model and input data, the GLUE analysis show that the total sampled copper mass can be predicted within a range of $\pm 50\%$ of the median value (385 g), whereas the grey-box analysis showed a prediction uncertainty of less than $\pm 30\%$. Future work will clarify the pros and cons of the two methods and furthermore explore to what extent the estimation can be improved by modifying the underlying accumulation-washout model.

Keywords GLUE; grey-box modelling; stochastic differential equations; stormwater pollution; uncertainty

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Introduction

Mathematical simulation models are increasingly used to calculate pollutant loads to receiving waters as a basis for engineering decisions. Many approaches to pollutant load modelling exist, ranging from simple regression models to continuous time process models accounting for accumulation-washout phenomena, but it is not always easy to determine if using a more complex models produce results that are worth the effort required to make them operational (Vaze and Chiew, 2003). Indeed, all models are associated with a significant amount of prediction uncertainty, which to a large extent is determined by the availability of data for calibration and verification (Bertrand-Krajewski, 2007). A further complicating factor lies in the choice of methods for uncertainty assessment, as different methods exist for estimation the prediction uncertainty (e.g. Lei, 1996).

In this paper we focus on determining the uncertainty associated with estimating the copper load from a stormwater system given a conceptual stormwater quality model and a, in this context, relatively detailed measurement campaign. The motivation for determining this is to investigate to what extent micro-pollutant loads in stormwater systems can be estimated. As a reference compound, the heavy metal copper was selected due to its abundance in building materials, its confirmed presence in dry and wet deposition and its confirmed aquatic toxicity and accumulation in e.g. river sediments (i.e. Eriksson *et al.*, 2007). Two attempts to assess the uncertainty involved with predicting pollutant loads from stormwater systems are made using methods that are increasingly used and well described in the literature. Both attempts include the application of results from a

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measurement campaign (rainfall, runoff volumes and pollutant masses) and a conceptual stormwater accumulation-washout model.

In the first attempt, the generalized likelihood uncertainty estimation (GLUE) methodology of Beven and Binley (1992) is applied. In this method model structure, input data, and parameter uncertainty are taken into account by accepting that there is no single correct optimal parameter set in an environmental modeling calibration study. Instead, model parameter sets that result in model output distributions encompassing a significant number of the measurements are derived.

In the second attempt, the conceptual model is re-formulated into a system of stochastic differential Equations (SDEs) by adding an additive noise term to the derivatives of the deterministic model. This technique is often referred to as grey-box modeling (i.e. Harremoës and Madsen, 1999). The idea is to take into account model structure approximations, unrecognized or un-modeled inputs and errors in the input data explicitly in the model equations. The parameters of the SDE system can then be estimated by means of maximum-likelihood estimation. By analyzing the estimation results, it is possible to pin-point model structure deficiencies, to identify insignificant model parameters and to quantify the uncertainty of the parameter estimates. In this paper initial results from grey-box modeling of stormwater quality are given.

Material

Site description and field data

All physical data come from the Vasastaden urban catchment in the city of Göteborg, Sweden. The catchment is densely populated and consists mainly of older residential and commercial buildings. The catchment has a total impervious area of 4.83 ha and a separate sewer system. For a detailed description of the case study see Ahlman (2006).

Measurements of rainfall, stormwater flow and stormwater quality were undertaken in April-May 2002. An ISCO 6700 automatic water sampler was installed in the vicinity of a manhole to take samples in a 400 mm separate storm sewer made out of concrete. A flow meter forced the sampler to take flow-weighted samples. Rain data was collected with a tipping bucket rain gauge (type HoBo/MJK), located approximately 60 m from the sampler on the boundary of the catchment.

Thirteen rainfall-runoff events during a period of 30 days were identified for analysis. The rainfall for these events ranged between 0.8 and 11.7 mm with durations from 0.4 to 9.7 hours. The maximum intensities (with a one-minute resolution) ranged between 0.4 and 3.7 mm/h. Within 8 hours after each rain event, the collected stormwater samples were transported to the laboratory where they were analyzed for pH, conductivity, total suspended solids (TSS), chemical oxygen demand (COD) and heavy metals (copper, zinc, lead and cadmium); in this paper only copper is in focus. The 13 events included analyses of 57 copper concentrations, which were representative for 57 runoff volumes.

Model description

We apply a conceptual rainfall-runoff and pollutant accumulation-washout model, similar to the one of Ahlman (2006) to simulate the load of copper in the stormwater. In the considered model pollutants are accumulated in dry periods and washed out during rainfall, processes described with classical build-up and wash-off functions (Overton and Meadows 1976). The model is illustrated in Figure 1 and explained below.

The effective rain intensity (i.e. the rain remaining after subtraction of initial loss) p_{eff} [m/s], the runoff coefficient ϕ [-], reservoir coefficient K [$\mathrm{m}^{3/5}\cdot\mathrm{s}^{-1}$] (representative for the hydrologic delay) and impervious area A [m^2] have been calibrated in a previous

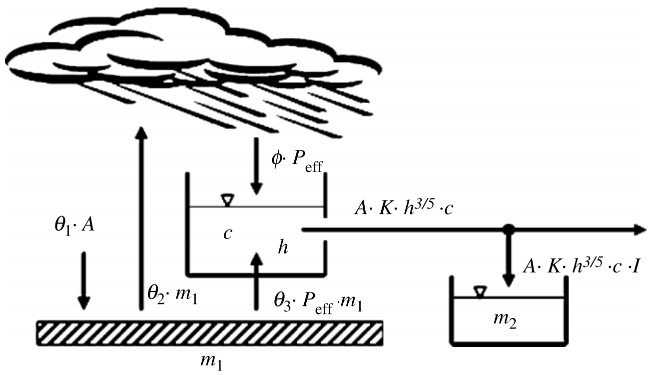

Figure 1 The conceptual stormwater rainfall-runoff and accumulation-washout model

study (Ahlman *et al.,* in prep.). These parameters are considered to be fixed and are not further analyzed.

The dry deposition load θ_1 [$\mathrm{g\,s^{-1}\,m^{-2}}$] is assumed to be constant and represents different sources of pollution, e.g. traffic activities, surface corrosion and atmospheric deposition. The concentration of copper in rain water has been neglected since it is low compared to the contribution from dry deposition. The rate coefficient for pollutant dry removal θ_2 [$\mathrm{s^{-1}}$] describes removal by wind and other means, a process which is assumed to be proportional to the accumulated mass m_1 [g]. The wet removal by wash-off is assumed to be proportional to m_1 and p_{eff} with a rate constant θ_3 [$\mathrm{m^{-1}}$]. Pollutants are mixed with rain in a hypothetical reservoir with dynamic storage h [m] to yield the stormwater pollutant concentration c [$\mathrm{g/m^3}$]. The pollution in runoff is then sampled and summed up to form the accumulated pollutant mass m_2 [g]. I is a function indicating when the flow-proportional samples are taken. The conceptual model is given by the following ordinary differential Equations (ODEs):

$$\frac{\mathrm{d}h}{\mathrm{d}t} = \phi \cdot p_{\text{eff}} - K \cdot h^{3/5} \tag{1}$$

$$\frac{\mathrm{d}c}{\mathrm{d}t} = \frac{p_{\text{eff}}}{h \cdot A} \cdot (\theta_3 \cdot m_1 - c \cdot \phi \cdot A) \tag{2}$$

$$\frac{\mathrm{d}m_1}{\mathrm{d}t} = A \cdot \theta_1 - (\theta_2 + \theta_3 \cdot p_{\text{eff}}) \cdot m_1 \tag{3}$$

$$\frac{\mathrm{d}m_2}{\mathrm{d}t} = A \cdot K \cdot h^{3/5} \cdot c \cdot I \tag{4}$$

Method

Sampling

The information obtained from the sampling campaign was used to form an observation vector $\boldsymbol{y}$, the cumulative masses of copper in the runoff. With $\boldsymbol{x}_t = [h\ c\ m_1\ m_2]$ denoting the state variables, $\boldsymbol{u}_t = [p_{\text{eff}}\ I]$ the input data and $\boldsymbol{\theta} = [\theta_1\ \theta_2\ \theta_3]$ the parameter vector to be analyzed, Equations (1)–(4) can be written in the compact from:

$$\frac{\mathrm{d}x_t}{\mathrm{d}t} = \boldsymbol{f}(\boldsymbol{x}_t, \boldsymbol{u}_t, t, \boldsymbol{\theta}) \tag{5}$$

with the observation equation:

$$y_k = m_{2,k} + e_k \tag{6}$$

where e_k ($k = 1, \ldots, 57$) denotes the difference between simulated ($m_{2,k}$) and observed (y_k) output at sampling instance k.

The Generalized Likelihood Uncertainty Estimation (GLUE) approach

The GLUE analysis in this paper is briefly described below. For a more dense discussion of the current application see Lindblom *et al.* (2007).

(1) Define the *prior distribution,* including information about the parameters before obtaining the observed data. Here, as well as in most GLUE applications, this is assumed to be a hypercube distribution.

(2) Draw $b = 1, 2 \ldots, B$ parameter sets from the prior distribution and simulate the residuals with the model in Equations (1)–(4) and (6).

(3) Calculate the associated B likelihoods. Here, likelihood is treated in a less formal way than in e.g. maximum likelihood theory and is denoted L_{GLUE}. Out of several likelihood functions used in GLUE studies (e.g. Beven and Freer, 2001), we applied:

$$L_{\text{glue}}(\boldsymbol{y}|\boldsymbol{\theta}^b) = \exp\left(-\frac{\sum_{k=1}^{57}(e_k^b)^2}{T}\right) \tag{7}$$

where T is a scaling parameter that can be tuned to determine the "wideness" of the distribution of the generated output.

(4) Normalize the likelihoods so that they sum up to one:

$$P^b = \frac{L_{\text{glue}}(\boldsymbol{y}|\boldsymbol{\theta}^b)}{\sum_{b=1}^{B} L_{\text{glue}}(\boldsymbol{y}|\boldsymbol{\theta}^b)} \tag{8}$$

(5) Finally, for each sampling instance k, the accumulated mass predicted by each parameter set is ranked in order of magnitude, and using the weights P^b associated with each set, a distribution function of the prediction is calculated.

The grey-box modelling approach

The ODE model (5) is transformed to a so called Itô stochastic differential Equation (SDE) model as:

$$\mathrm{d}\boldsymbol{x}_t = \boldsymbol{f}(\boldsymbol{x}_t, \boldsymbol{u}_t, t, \boldsymbol{\theta})\mathrm{d}t + \boldsymbol{\sigma}_t \mathrm{d}\boldsymbol{\omega}_t \tag{9}$$

where $\boldsymbol{\omega}_t$ is a standard Wiener process. The observation Equation (Equation 6) remains unchanged. Compared to the model given by (5), (9) contains additional parameters inside the matrix $\boldsymbol{\sigma}_t$. This paper is strictly focused on the pollutant deposition-washout process and how it is modeled (Equation 3) and thus we included only one additional parameter (σ_{33}) in the third diagonal element of $\boldsymbol{\sigma}_t$. The remaining elements in the matrix consist of zeros.

Parameter estimation in grey-box modeling. We used the software *CTSM* (Kristensen and Madsen, 2003) to estimate the parameters in (9). This is done according to maximum likelihood estimation theory. The basis for this theory is given below. For a more detailed description see Kristensen *et al.* (2004). With Y_N being a vector containing all the observations up to and including N, the likelihood function is the joint probability density of all the observations taken as a function of $\boldsymbol{\theta}$:

$$L(\boldsymbol{\theta}; Y_N) = \left(\prod_{k=1}^{N} p(y_k | Y_{k-1}, \boldsymbol{\theta})\right) p(y_1 | y_0, \boldsymbol{\theta}) \tag{10}$$

Since the increments of the Wiener process ***w(t)*** are approximately Gaussian, the conditional densities in (10) can be assumed to be normal. Hence, in order to parameterize the conditional distribution, the conditional mean and conditional variance are introduced:

$$\hat{y}_{k|k-1} = E[y_k | Y_{k-1}, \boldsymbol{\theta}] \tag{11}$$

$$R_{k|k-1} = V[y_k | Y_{k-1}, \boldsymbol{\theta}] \tag{12}$$

It is also convenient to introduce the one-step prediction error:

$$\varepsilon_k = y_k - \hat{y}_{k|k-1} \tag{13}$$

With this notation the likelihood function can be written:

$$L(\boldsymbol{\theta}; Y_N) = \left(\prod_{k=1}^{N} \frac{\exp(-(1/2)\varepsilon_k^2 R_{k|k-1})}{\sqrt{R_{k|k-1}}\sqrt{2\pi}}\right) \tag{14}$$

CTSM calculates the conditional mean and the conditional variance recursively by using the extended Kalman filter. The maximum-likelihood estimate (ML-estimate) is then given by the parameter set $\hat{\boldsymbol{\theta}}$, which maximizes the likelihood function. Note that $\boldsymbol{\theta}$ here includes both the three accumulation-washout parameters, as well as σ_{33} and the residual variance σ_e^2. The optimization problem is solved numerically by the quasi-Newton method. In this work *CTSM* was used to find the parameter estimate $\hat{\boldsymbol{\theta}}$ and then to provide output estimates based only on the inputs, i.e. $\hat{y}_{k|0}$, along with their standard deviations S.D. $(\hat{y}_{k|0})$.

Results and discussion

GLUE analysis

The selected minimum and maximum parameter values defining the prior (hypercube) distribution are shown in Table 1. First 50,000 simulations according to step (1) and (2) mentioned above were conducted. Steps (3)–(5) were then iterated with various values of the scaling parameter T. With $T = 4 \times 10^5$, we judged that the uncertainty was adequately described; all 57 data were covered by the 95% bands. The obtained distributions are shown as box-plots (95% and 50% quantiles) in Figure 2. For $k = 3$ and $k = 26$ the observations show a significant "jump" due to abnormally high observed mass in the observations, which are not simulated well by the model. This pattern is for $k = 3$ due to the so-called "first flush" phenomenon occasionally leading to very high initial runoff concentrations after long dry spells, which may be better simulated using an exponent in

Table 1 Minimum and maximum parameter values defining the prior distribution in the Glue analysis and maximum likelihood estimates from the grey-box modeling

Parameter	Unit	Min	Max	ML-estimate
θ_1	(g s^{-1} m^{-2})	1×10^{-9}	1×10^{-7}	8.9×10^{-9}
θ_2	(s^{-1})	1×10^{-7}	1.5×10^{-4}	5.7×10^{-6}
θ_3	(m^{-1})	0	1×10^{4}	4.2×10^{2}
σ_{33}	(g/s)	–	–	8.6×10^{-2}
σ_e	(g)	–	–	1.9

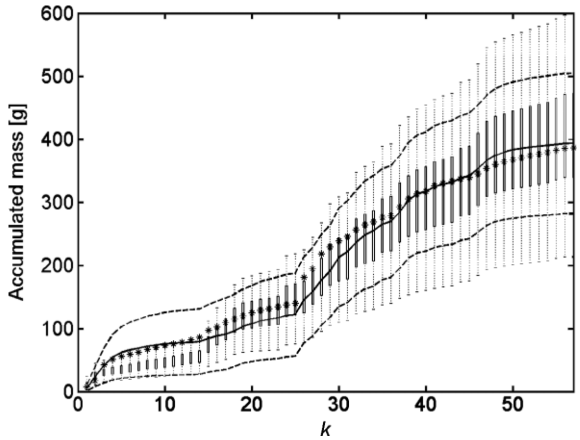

Figure 2 Asterisks: The cumulative sum of the measured copper masses (y_k). Boxes: Distributions from the GLUE-analysis (95% and 50% quantiles). Solid line: ML-estimate of the grey-box model. Dashed lines: 95% confidence limit for ML-estimate of the grey box model

p_{eff} in the formulation of the washout process (Equation 3), as originally proposed by Overton and Meadows (1976). For $k = 26$ there is no easy explanation; the pattern may be caused by sample contamination or measurement errors, which means the observation should be treated as an outlier and not be used in the GLUE process. In this paper we have not attempted to modify the model to obtain a better fit with data, and all data that were not rejected in the usual quality assurance were included. Rather, we have focused on determining the uncertainty given a fixed model and data set by tuning T to practically cover all observations. This leads to a relatively high uncertainty estimate; the total copper mass can only be estimated with an uncertainty of $\pm 50\%$ of the median (385 g).

Grey box modeling

In Table 1, the obtained maximum likelihood estimates of the parameters from the grey box modeling are shown. In Figure 2 the corresponding output estimates are shown (solid line) together with the 95% confidence bounds ($\hat{y}_{k|0} \pm 1.96 \cdot \mathrm{S.D.}\ (\hat{y}_{k|0})$). It is noted that the three ML parameter estimates $\boldsymbol{\theta} = [\theta_1\ \ \theta_2\ \ \theta_3]$ all are within the limits of the prior distributions defined for the GLUE analysis.

The ML-estimate of the copper load follows the observations relatively closely in the whole sequence $k = 1, \ldots, 57$, and results in a lower uncertainty than the GLUE analysis; the total copper mass is in this case estimated with an uncertainty of $\pm 30\%$. The theory for maximum-likelihood estimation included in *CTSM,* and also briefly shown above, relies on the Gaussianity assumptions of the conditional means and variances as well as on white noise characteristics of the residuals. In this paper, no attempts to ensure that these assumptions are fulfilled have been made. The residuals do not seem, as shown in Figure 3, to be uncorrelated, nor to have a mean equal to zero. As pointed out in Kristensen *et al.* (2004), the assumptions are not likely to be valid when the model structure is not perfect, which is often the case in the initial phase of a grey-box modeling procedure. However, in such cases the estimation results can be used to provide indications for model improvement. Maximum likelihood estimates of the grey-box model parameters showed that the parameter σ_{33} was significant, i.e. not zero. Thus it was pin-pointed that this part of the model must be considered to be uncertain and perhaps also re-formulated. The results also showed that σ_{33} was significant compared to the residual variance σ_e, i.e. the deviation between measured and simulated data cannot be solely explained by measurement errors.

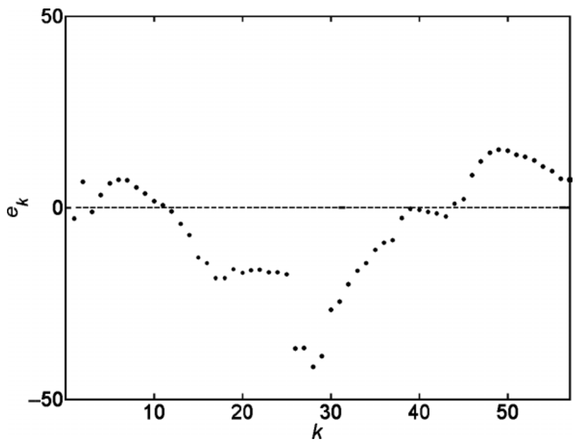

Figure 3 Residuals from the grey-box simulation

The results show that the GLUE and the grey-box method yield very similar results in terms of the median/mean, but that the GLUE method provides a substantially higher uncertainty estimate. This difference is perhaps not surprising, since the two methods are based on different assumptions (e.g. with respect to error structure) and developed for different purposes (i.e. GLUE to estimate the uncertainty of existing models, grey-box modeling to improve models especially in a predictive on-line context). The exact causes are however not clear at this stage. Future work will clarify the pros and cons of the two methods and furthermore explore to what extent the estimation can be improved by modifying the underlying accumulation-washout model or accounting for speciation of the suspended pollutant mass between the solid and dissolved forms. The conclusions are however expected to depend on the amount and quality of the available data, and perhaps also on the inherent properties of the studied micropollutants. Therefore, it cannot be excluded that simpler models, for example event-lumped, based on daily loads or purely stochastic may be appropriate in some cases.

Conclusions

Given an extensive measurement campaign and an accumulation-washout model describing dynamic variations in runoff concentrations, it is concluded that the estimation of micro-pollutants in stormwater is associated with significant uncertainty. With the proposed model and input data, a GLUE analysis show that the total sampled copper mass can be predicted within a range of $\pm 50\%$ of the median value (385 g). By reformulating the deterministic model into a grey-box model followed by a maximum likelihood estimation of the parameters, the obtained model output uncertainty was determined to be lower and $\pm 30\%$. Future work will clarify the pros and cons of the two methods and furthermore explore to what extent the estimation can be improved by modifying the underlying accumulation-washout model.

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