

**Improving
uncertainty
estimation in urban
hydrology**

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Improving uncertainty estimation in urban hydrological modeling by statistically describing bias

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Abstract

Hydrodynamic models are useful tools for urban water management. Unfortunately, it is still challenging to obtain accurate results and plausible uncertainty estimates when using these models. In particular, with the currently applied statistical techniques, flow predictions are usually overconfident and biased. In this study, we present a flexible and computationally efficient methodology (i) to obtain more reliable hydrological simulations in terms of coverage of validation data by the uncertainty bands and (ii) to separate prediction uncertainty into its components. Our approach acknowledges that urban drainage predictions are biased. This is mostly due to input errors and structural deficits of the model. We address this issue by describing model bias in a Bayesian framework. The bias becomes an autoregressive term additional to white measurement noise, the only error type accounted for in traditional uncertainty analysis in urban hydrology. To allow for bigger discrepancies during wet weather, we make the variance of bias dependent on the input (rainfall) or/and output (runoff) of the system. Specifically, we present a structured approach to select, among five variants, the optimal bias description for a given urban or natural case study. We tested the methodology in a small monitored stormwater system described by means of a parsimonious model. Our results clearly show that flow simulations are much more reliable when bias is accounted for than when it is neglected. Furthermore, our probabilistic predictions can discriminate between three uncertainty contributions: parametric uncertainty, bias (due to input and structural errors), and measurement errors. In our case study, the best performing bias description was the output-dependent bias using a log-sinh transformation of data and model results. The limitations of the framework presented are some ambiguity due to the subjective choice of priors for bias parameters and its inability to directly reduce the causes of bias. More experience with the application of this framework will lead to a greater prior knowledge for a bias formulation. Furthermore, propagation of input uncertainty and improvement to the model structure are expected to reduce the bias.

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1 Introduction

Mathematical simulation models play an important role in the design and assessment of urban drainage systems. On the one hand, they are used to investigate the current system, for example regarding the capacity for and likelihood of flooding. On the other hand, engineers use them to predict the consequences of future changes of boundary conditions or control strategies (Gujer, 2008; Kleidorfer, 2009; Korving and Clemens, 2005). Traditionally, according to standards of good engineering practice, such models were calibrated by adjusting in parameters in such a way as to allow predicted flows to closely reflect field data. In recent years, it has been recognized that predictions of urban drainage models are not of much practical use without an estimate of their uncertainty (Dotto et al., 2011; Kleidorfer, 2009; Korving and Clemens, 2005). Unfortunately, there are so far no established methods available to assess prediction uncertainty in sewer hydrology in a statistically satisfactory way (Freni et al., 2009b; Breinholt et al., 2012).

Most studies in urban hydrology compute uncertainty intervals of sewer flows by simply propagating model parameter uncertainty and adding independent measurement errors to the output, often by means of Monte Carlo simulation (e.g. Dotto et al., 2011; Freni et al., 2009b). However, an independent error term makes only sense if the random measurement errors would be the dominating source of uncertainty. Additionally, it would be desirable that a random realization of the error model results in a trajectory that is in agreement with observed data. Unfortunately, this is not the case with iid errors.

In the context of design, operation and assessment of urban hydrosystems, it is important to obtain reliable predictions from a calibrated model (Sikorska et al., 2012). This means that random draws from the model should have similar statistical properties (such as variance or autocorrelation) as the data. Additionally, for reliable predictions, the observed coverage of the simulated uncertainty bounds should match or exceed the nominal coverage. Ideally, this can be achieved by representing the dominant

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model bias is present in virtually every study and (ii) there is a great need to abandon the traditional assumption of random measurement errors in urban drainage, as in most other environmental modeling studies also. Instead, all uncertainty components must be captured in a statistically rigorous manner to avoid overconfident flow predictions.

To better fulfill the statistical assumptions of homoskedasticity and normality of calibration residuals, and so obtain more reliable predictions, it is a common practice in hydrology to transform simulation results and output data (Schoups and Vrugt, 2010). The Box-Cox transformation (Box and Cox, 1964) has indeed been successfully used in several case studies, both rural (e.g. Frey et al., 2011; Honti et al., 2013; Reichert and Mieleitner, 2009; Yang et al., 2007b,a; Sikorska et al., 2012) and urban (e.g. Dotto et al., 2011; Freni et al., 2009b; Breinholt et al., 2012). Admittedly, transformation stabilizes the variance of the residual errors in the transformed space. Unfortunately, it has almost no effect on the serial autocorrelation of residuals and thus cannot capture model bias.

To account for systematic deviations of model results from field data, it seems promising to apply autoregressive error models that lump all uncertainty components into a single process (Kuczera, 1983; Bates and Campbell, 2001; Yang et al., 2007b; Schoups and Vrugt, 2010). Such models are not only relatively straightforward to apply, but also often help to meet the underlying statistical assumptions. However, a disadvantage of such lumped error models is that only parameter uncertainty can be separated from the total predictive uncertainty. To additionally separate bias from random measurement errors, Kennedy and O'Hagan (2001), Higdon et al. (2005), Bayarri et al. (2007) and others suggested using a Gaussian stochastic process to describe the knowledge about the bias with an independent error term for observation error. This approach has been applied to environmental modeling and linked to multi-objective model calibration by Reichert and Schuwirth (2012). Recently, a more complex input-dependent description of bias has been applied successfully by Honti et al. (2013). In their study, this solved the problem that the structural error was greater during rainy periods than during dry weather, a common situation in hydrology (Breinholt et al., 2012).

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Going in a different direction of error separation, Sikorska et al. (2012) combined the lumped autoregressive error model with rainfall multipliers to separate the effect of input uncertainty from (lumped, remaining) bias and flow measurement errors.

In summary, there are three major interrelated needs in (urban) hydrological modeling: (i) to obtain reliable predictions, (ii) to disentangle prediction uncertainty into its components, and (iii) to fulfill the statistical assumptions behind model calibration. In particular, need (iii) is necessary to fulfill requirements (i) and (ii) in a satisfying way.

To address the issues mentioned, here we adapt the framework of Kennedy and O'Hagan (2001) as formulated by Reichert and Schuwirth (2012) to assess model bias along with other uncertainty components. This makes it possible to provide reliable predictions of (urban) hydrological models while meeting the underlying statistical assumptions. At the same time, this approach takes into consideration different uncertainty components, namely output measurement errors, parametric uncertainty and the effect of structural deficits and input measurement errors on model output. With this approach all uncertainties are described in the output. This does not allow separating among input errors and structural deficits. However, a statistical bias description is simpler and less computationally intensive than approaches addressing the causes of bias via mechanistic propagation of rainfall uncertainty (Renard et al., 2011), stochastic time-dependent parameters (Reichert and Mieleitner, 2009), or by combining filtering and data augmentation (Bulygina and Gupta, 2011).

Although focused on urban settings, our methodology is also suitable in other contexts like natural watersheds, where generally processes occur on longer time scales and output measurements are more uncertain. In this paper, we do not advocate an ideal error model that fits every situation. In our view, although very desirable, such a model might be unrealistic because watershed behaviors, measurement strategies and hydrodynamic models differ from case to case. Instead, we suggest a structured approach for finding the most suitable description of model bias for a given hydrosystem and a given deterministic model.

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Specifically, we investigate different strategies to parameterize the bias description by (i) making it input-dependent and (ii) making it output-dependent by applying two different transformations. The distinguishing innovations of our study are:

- i. A formal investigation of model bias in urban hydrology. This makes it possible to obtain reliable uncertainty intervals of sewer flows, also because the underlying statistical assumptions have not been violated.
- ii. An assessment of the importance of model bias by separating prediction uncertainty into the individual contributions of bias, effect of model parameter uncertainty and measurement errors.
- iii. A systematic comparison of different bias formulations and transformations. This is highly relevant for both natural and urban hydrology because we can acquire knowledge for potential future studies.
- iv. An assessment of predictive uncertainties of flows for past (calibration) and future (extrapolation) system states. We find that considering bias not only produces reliable prediction intervals. It also accounts for increasing uncertainty when flow predictions move from observed past into unknown future conditions. Furthermore, we discuss how the exploratory analysis of bias and monitoring data can be used to improve the hydrodynamic model.

The remainder of this article is structured as follows: first, we present the statistical description of model bias and compare it to the classical approach. Second, we introduce two different bias formulations and two transformations, and describe how we evaluate the performance of the resulting runoff predictions. Third, we test our approach on a high-quality dataset from a real-world stormwater system in Prague, Czech Republic, and present the results obtained with the different error models. Fourth, we discuss these results as well as advantages and limitations of our approach based on theoretical reflections and our practical experience. In addition, we suggest how to

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select the most appropriate error formulations for urban and also natural hydrological studies and outline future research needs.

2 Methods

2.1 Likelihood function

5 To statistically estimate the predictive uncertainty of urban drainage models, we need a likelihood function (a.k.a. sampling model), $f(\mathbf{y}_o | \xi, \mathbf{x})$, which combines (in this particular case) a deterministic model (a.k.a. simulator), M , with a probabilistic error term. $f(\mathbf{y}_o | \xi, \mathbf{x})$ describes the joint probability density of observed system outcomes, \mathbf{y}_o , given the model parameters, ξ , and external driving forces, \mathbf{x} , such as precipitation.

10 The probability density, $f(\mathbf{y}_o | \xi, \mathbf{x})$, may have a frequentist (describes a limiting distribution of a large number of observations) or a Bayesian (describes knowledge or belief) interpretation. Only frequentist elements in a likelihood function can be empirically tested. To formulate such a likelihood function, we need (i) a simulator of the system with parameters θ , and (ii) a stochastic model of the errors with parameters ψ .

15 During calibration (a.k.a. parameter inference), the joint probability density of parameter and model results, proportional to the product of the prior of the parameters and the likelihood, $f(\mathbf{y}_o | \xi, \mathbf{x})$, is conditioned on the data to derive a joint posterior for both deterministic model and error model parameters, i.e. $\xi = (\theta, \psi)$.

20 A generic likelihood function assuming a multivariate Gaussian distribution with covariance (or dispersion) matrix $\Sigma(\psi, \mathbf{x})$ of output transformed by a transformation $g()$ can be written as:

$$f(\mathbf{y}_o | \theta, \psi, \mathbf{x}) = \frac{(2\pi)^{-\frac{n}{2}}}{\sqrt{\det(\Sigma(\psi, \mathbf{x}))}} \exp\left(-\frac{1}{2} [\tilde{\mathbf{y}}_o - \tilde{\mathbf{y}}_M(\theta, \mathbf{x})]^T \Sigma(\psi, \mathbf{x})^{-1} [\tilde{\mathbf{y}}_o - \tilde{\mathbf{y}}_M(\theta, \mathbf{x})]\right) \prod_{i=1}^n \frac{dg}{dy}(y_{o,i}, \psi), \quad (1)$$

where n is the number of observations, i.e. the dimension of \mathbf{y}_o , which could be, for instance, a sewer flow time series. \mathbf{y}_M are the corresponding model predictions. The tilde denotes transformed quantities, i.e. $\tilde{\mathbf{y}} = g(\mathbf{y})$. Note that Eq. (1) assumes the residual errors to have 0 as expected value.

Uncertainty analysis for predictions is usually preceded by model calibration during which the parameters of both the hydrological model, θ , and the error model, ψ , are inferred. This parameter inference procedure requires that the statistical assumptions underlying the likelihood function be approximately fulfilled. This means that the Bayesian part of the likelihood function should correctly represent (conditional) knowledge/belief of the analyst (given the model parameters). This assumption is not testable. In contrast, frequentist assumptions can be tested by comparing empirical distributions with model assumptions. In our error models, we will have a frequentist interpretation of the observation error that can be tested, whereas the distributional assumption of the bias cannot be tested. If frequentist assumptions are violated, options are (i) to improve the structure of the deterministic model, (ii) to modify the distributional assumptions, or (iii) to improve the error model, e.g. by using a statistical (Bayesian) bias description.

- i. In environmental modeling, improving the model structure, e.g. by a more detailed description of relevant processes or by increasing the spatial resolution, can reduce, but not eliminate the bias. Natural systems are so complex that models will always be a simplified abstraction of the physical reality, unable to describe natural phenomena without bias. In addition, increasing model complexity will increase parametric uncertainty and computation time. Input errors are relevant when dealing with highly variable forcing fields, as is the case for precipitation. Having a denser point measurement network or combining different types of input observations (e.g. from pluviometers, radar and microwave links) can reduce this uncertainty. However, for practical reasons, input errors cannot be completely eliminated (Berne et al., 2004).

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ii. A simple way of improving the distributional assumptions is applying a transformation to model results and data and applying the convenient distributional assumptions to the transformed values. This technique is commonly applied in hydrology to reduce heteroscedasticity and skewness of (random observation) errors, while simultaneously accounting for increasing uncertainty during high flow periods (Wang et al., 2012; Breinholt et al., 2012). Alternatively, a similar effect can be achieved through heteroscedastic error models with error variance dependent on external forcings (Honti et al., 2013) or simulated outputs (Schoups and Vrugt, 2010).

iii. To account for difficult-to-reduce input and structural errors responsible for auto-correlated residuals, it has been suggested to describe prior knowledge of model bias by means of a stochastic process and to update this knowledge through conditioning with the data (Craig et al., 2001; Kennedy and O'Hagan, 2001; Higdon et al., 2005; Bayarri et al., 2007).

To increase the reliability of our probabilistic predictions and the fulfillment of the underlying assumptions for a given model, we will focus here on combining the strategies (ii) and (iii).

In the following paragraphs, we will consider nine different likelihood functions by systematically modifying (i) the dispersion matrix of the residuals Σ (Sects. 2.1.1 and 2.1.2) and (ii) the transformation function g (Sect. 2.1.3). Three forms of parameterization of the bias process will be considered: neglect of bias (traditional error model with independent observation errors only), a stationary bias process, and an input-dependent bias process. Regarding output transformation, we compare the identity (no transformation), the Box-Cox transformation, and a recently suggested log-sinh transformation (references are given below).

2.1.1 Independent error model

In urban hydrology, the most commonly used statistical technique to estimate predictive uncertainty assumes an independent error model (Dotto et al., 2011; Freni et al., 2009a; Breinholt et al., 2012). Besides the absence of serial correlation, this requires residual errors identically distributed around zero.

The transformed observed system output, \tilde{Y}_o , is modelled as the sum of a deterministic model output $\tilde{y}_M(\mathbf{x}, \boldsymbol{\theta})$ and an error term representing the measurement noise of the system response E

$$\tilde{Y}_o(\mathbf{x}, \boldsymbol{\theta}, \boldsymbol{\psi}) = \tilde{y}_M(\mathbf{x}, \boldsymbol{\theta}) + E(\boldsymbol{\psi}) \quad , \quad (2)$$

where variables in capitals are random, whereas those in lowercase are deterministic.

Assuming independent identically distributed normal errors in the transformed space, E follows a multivariate normal distribution with mean 0 and a diagonal covariance matrix,

$$\boldsymbol{\Sigma}_E = \sigma_E^2 \mathbf{1} \quad . \quad (3)$$

We then have $\boldsymbol{\psi} = \sigma_E$, and the covariance matrix of Eq. (1) is given by $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}_E$. As $E(\boldsymbol{\psi})$ is interpreted to represent observation error, the distributional assumptions are testable through residual analysis. Note that while in hydrology the observation and measurement errors are used as synonyms, in other environmental contexts observation errors can contain additional sampling errors.

2.1.2 Autoregressive bias error model

In contrast to the independent error model, the autoregressive bias error model explicitly acknowledges the fact that simulators cannot describe the “true” behaviour of a system. This has been originally suggested in the statistical literature (Craig et al., 2001; Kennedy and O’Hagan, 2001; Higdon et al., 2005; Bayarri et al., 2007) and later adapted to environmental modelling (Reichert and Schuwirth, 2012).

Technically, model inadequacy (also called bias or discrepancy) is considered by augmenting the independent error model with a bias term:

$$\tilde{Y}_o(\mathbf{x}, \boldsymbol{\theta}, \boldsymbol{\psi}) = \tilde{y}_M(\mathbf{x}, \boldsymbol{\theta}) + \mathbf{B}_M(\mathbf{x}, \boldsymbol{\psi}) + \mathbf{E}(\boldsymbol{\psi}) \quad . \quad (4)$$

On the one hand, this model bias \mathbf{B}_M can capture the effect of errors in input measurements and structural limitations. On the other hand, it can also describe systematic output measurement errors, e.g. from sensor failure, incorrectly calibrated devices or erroneously estimated rating curves. In its simplest form, the bias is modelled as an autocorrelated stationary random process (Reichert and Schuwirth, 2012). However, it can also have a more complex structure and, for instance, be input-dependent (Honti et al., 2013). Notice that, rigorously speaking, \mathbf{B}_M represents a bias-correction whereas the bias itself is its negative.

Conceptually, one difficulty is the identifiability problem between model and bias, which is apparent in Eq. (4). As both cannot be observed separately, this issue can only be solved by considering prior knowledge on the bias in parameter estimation. This requires a Bayesian framework for inference and prior distributions that favour the smallest possible bias. Indeed, we desire output dynamics to be described as accurately as possible by the simulator and only the remaining deviations by the bias. Note that the distribution of the residuals, $\mathbf{B}_M(\mathbf{x}, \boldsymbol{\psi}) + \mathbf{E}(\boldsymbol{\psi})$, is not testable due to the Bayesian interpretation of $\mathbf{B}_M(\mathbf{x}, \boldsymbol{\psi})$. However, when estimating both $\mathbf{B}_M(\mathbf{x}, \boldsymbol{\psi})$ and $\mathbf{E}(\boldsymbol{\psi})$, the assumptions regarding the observation error, $\mathbf{E}(\boldsymbol{\psi})$, can be tested by frequentist tests.

Practically, the choice of an adequate bias formulation is challenging. On the one hand, examples from urban hydrological applications are currently lacking. On the other hand, the bias results from the complex interplay between the drainage system, the simulator and the monitoring data. This is not straightforward to assess a priori. Notice that the autocorrelated bias and the random observation errors are usually well distinguished from each other by virtue of their distinct statistical properties.

In the following, we investigate four different bias formulations: (i) input and output-independent (i.e., constant), (ii) output-dependent, (iii) input-dependent, (iv) input and

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output-dependent. The constant bias is modeled via a standard Ornstein-Uhlenbeck (OU) process. The output-dependence is considered through transformation of measured and simulated data. The input-dependence uses a modified OU process, which is perturbed by rainfall.

5 Input-independent bias

The simplest bias formulation is a mean-reverting Ornstein-Uhlenbeck (OU) process (Uhlenbeck and Ornstein, 1930), the discretization of which would be a first-order autoregressive process (AR(1)) with iid noise. The OU process is a stationary Gauss-Markov process with a long-term equilibrium value of zero and a constant variance, either in the original or transformed space. The one-dimensional OU process B_M is described by the stochastic differential equation

$$dB_M(t) = -\frac{B_M(t)}{\tau}dt + \sqrt{\frac{2}{\tau}}\sigma_{B_{ct}}dW(t) \quad , \quad (5)$$

where τ is the correlation time and $\sigma_{B_{ct}}$ is the asymptotic standard deviation of the random fluctuations around the equilibrium. $dW(t)$ is a Wiener (white noise) process which is the same as standard Brownian motion. For an introduction on stochastic processes see, e.g., Iacus (2008); Henderson and Plaschko (2006); Kessler et al. (2012).

This stationary bias results in the likelihood function of Eq. (1) with covariance matrix $\Sigma = \Sigma_E + \Sigma_{B_M}$ with

$$\Sigma_{B_M,i,j}(\boldsymbol{\psi}) = \sigma_{B_{ct}}^2 \exp\left(-\frac{1}{\tau}|t_i - t_j|\right) \quad . \quad (6)$$

In contrast to the formulation given by Eq. (6), the covariance in the original formulation by Kennedy and O'Hagan (2001) had an exponent α for the term $|t_i - t_j|$. To guarantee differentiability, this exponent is often chosen to be equal to two. For hydrological applications we prefer an exponent of unity to be compatible with the OU process,

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which can be assumed to be a simple description of underlying mechanisms leading to a decay of correlation (Yang et al., 2007a; Sikorska et al., 2012). Indeed, such a covariance structure makes it possible to transfer the autoregressive error models (Kuczera, 1983; Bates and Campbell, 2001; Yang et al., 2007b) to the bias description framework.

5 Input-dependent bias

A more complex bias description considers input-dependency to mechanistically increase the uncertainty of flow predictions during rainy periods. Following Honti et al. (2013), we suggest an OU process whose variance grows quadratically with the precipitation intensity, x , shifted in time by a lag d . The equation for the rate of change of the input-dependent bias is then given by:

$$dB_M(t) = -\frac{B_M(t)}{\tau}dt + \sqrt{\frac{2}{\tau} \left(\sigma_{B_{ct}}^2 + (\kappa x(t-d))^2 \right)} dW(t) \quad , \quad (7)$$

where κ is a scaling factor and d denotes the response time of the system to rainfall. For an equidistant time discretization, with $t_{i+1} - t_i = \Delta t$, assuming that the lag is a constant multiple of Δt , $d = \delta \Delta t$, and the input is constant between time-points, we derive from Eq. (7) the recursion formula for the variance

$$E \left[B_M^2(t_i) \right] = E \left[B_M^2(t_{i-1}) \right] \exp \left(-\frac{2}{\tau} \Delta t \right) + \left[\sigma_{B_{ct}}^2 + (\kappa x_{i-\delta})^2 \right] \left(1 - \exp \left(-\frac{2}{\tau} \Delta t \right) \right) \quad . \quad (8)$$

The parameters $\boldsymbol{\psi}$ of this bias are given by

$$\boldsymbol{\psi} = (\sigma_{B_{ct}}, \tau, \kappa, d)^T \quad . \quad (9)$$

The resulting bias covariance matrix, $\boldsymbol{\Sigma}_{B_M}$, is given by

$$\boldsymbol{\Sigma}_{B_M, i, j}(\boldsymbol{\psi}, \mathbf{x}) = E \left[B_M^2(\min(t_i, t_j)) \right] \exp \left(-\frac{1}{\tau} |t_j - t_i| \right) \quad . \quad (10)$$

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In comparison to the original bias formulation by Honti et al. (2013), we modified two aspects. First, we consider the response time of the system by introducing a time lag of the input, which was necessary due to the high frequency of monitoring data. Indeed, instead of working with daily discharge data used in Honti et al. (2013), here we had 5 output observations every two minutes. Second, we omitted the fast bias component, which accounts for additional noise coming into action during the rainy timesteps. In our experience, this component did not have a significant effect at this short time scale and its elimination led to a greater simplicity and robustness of the error model.

2.1.3 Output transformation

In hydrological modeling, it is common practice to apply a transformation to account for augmented variance for large discharge. The two variance stabilization techniques which are, in our view, most promising for urban drainage applications are: the Box-Cox transformation (Box and Cox, 1964) and the log-sinh transformation (Wang et al., 10 2012).

Box-Cox

The Box-Cox transformation has been successfully used in many hydrological studies to reduce the output-dependence of the residual variance in the transformed space (e.g. Frey et al., 2011; Honti et al., 2013; Dotto et al., 2011; Reichert and Mieleitner, 2009; Yang et al., 2007b,a; Sikorska et al., 2012, 2013).

The one-parameter Box-Cox transformation can be written as:

$$g(y) = \begin{cases} \frac{y^\lambda - 1}{\lambda} & \text{if } \lambda \neq 0 \\ \log(y) & \text{if } \lambda = 0 \end{cases} \quad (11)$$

$$g^{-1}(z) = \begin{cases} (\lambda z + 1)^{1/\lambda} & \text{if } \lambda \neq 0 \\ \exp(y) & \text{if } \lambda = 0 \end{cases} \quad (12)$$

where g indicates the forward and g^{-1} the backward transformation. λ is a parameter that determines how strong the transformation is. It is chosen from the interval $[0, 1]$, with the extreme cases of 1 leading to the (shifted) identity transformation, 0 to a log transformation. Profiting from the experience in the literature (Willems, 2012; Honti et al., 2013; Yang et al., 2007b), we choose a value of $\lambda = 0.35$, which yields a moderate transformation that increases the variance for high discharges only to a degree that does not decrease their weight for calibration too strongly. The behavior of the Box-Cox transformation for the stormwater runoff in our study is shown in Fig. 1.

Log-sinh

The log-sinh transformation has recently shown very promising results for hydrological applications (Wang et al., 2012). In contrast to the original notation, we prefer a reparameterized form with more intuitive parameters:

$$g(y) = \beta \log \left(\sinh \left(\frac{\alpha + y}{\beta} \right) \right), \quad g^{-1}(z) = \left(\operatorname{arcsinh} \left(\exp \left(\frac{y}{\beta} \right) \right) - \frac{\alpha}{\beta} \right) \beta, \quad (13)$$

where α (originally a/b) and β (originally $1/b$) are lower and upper reference outputs, respectively. For outputs much smaller than α , the scaling of the error (derivative of g) is approximately constant, whereas for outputs larger than β , it is approximately equal to unity. In our case study, we chose α to be the minimal discharge below which the uncertainty does not further decrease and β to be the discharge above which uncertainty does not significantly increase. The characteristics of the catchment and the monitoring equipment suggested a setting of $\alpha = 5 \text{ L s}^{-1}$ and $\beta = 100 \text{ L s}^{-1}$. A graph of the transformation function with these parameter values is provided in Fig. 1.

Both transformations are able to reduce the heteroscedasticity of residuals, which represents the fact that flow meters and rating curves are more inaccurate during high flows and systematic errors lead to a higher uncertainty during high flows. Another positive characteristic is that these transformations make error distributions asymmetric,

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substantially reducing the proportion of negative flow predictions, which can otherwise occur during error propagation.

2.2 Inference and predictions

The following steps are needed to calibrate a deterministic model M with a statistical bias description and observation error and to analyze the resulting prediction uncertainties: (i) definition of the prior distribution of the parameters, (ii) obtaining the posterior distribution with Bayesian inference, (iii) probabilistic predictions for the temporal points (in the following called layout) used in calibration, (iv) probabilistic predictions for the extrapolation period. Finally, one has to assess the quality of the predictions and verify the statistical assumptions. We highly recommended an exploratory analysis of the bias, which can help to improve the structure of the simulator.

2.2.1 Prior definition

First, one has to define the joint prior distribution of the parameters of the hydrological model, θ , and of the error model, ψ . In particular, this requires an informative prior of the covariance matrix of the flow measurements. Although a first guess can be obtained from manufacturer's specifications, it is recommended to assess it separately with redundant measurements (see Dürrenmatt et al., 2013). As stated in Sect. 2.1.2, it is important that the prior of the bias reflect the desire to avoid model inadequacy as much as possible. This is obtained by a probability density decreasing with increasing values of $\sigma_{B_{ct}}$ and κ (e.g. an exponential distribution). This helps to reduce the identifiability problem between the deterministic model and the bias. For the prior for $\sigma_{B_{ct}}$, one could take into account that the maximum bias scatter is unlikely to be higher than the observed discharge variability. On the other hand, the maximum value of κ can hardly exceed the maximum discharge divided by the corresponding maximum precipitation of a previously monitored storm event. Additionally, τ should represent the characteristic correlation length of the residuals and could be approximately set

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to 1/3 of the hydrograph recession time. More prior information may be available from previous model applications to the same or a similar hydrological system. Finally, the parameters of the chosen transformation have to be specified.

We recognize that assigning priors for bias parameters might be challenging. Therefore we suggest testing a posteriori the sensitivity of the updated parameter distributions to the priors. We advise against using uniform improper priors for two reasons. First, as discussed above, our ignorance about bias parameters is not total. Second, as argued by Raiffa and Schlaifer (1961), if one lacks knowledge about ψ one should also lack knowledge about ψ^2 , but no distribution exists that is uniform on both ψ and ψ^2 (Christensen et al., 2010).

2.2.2 Bayesian inference

Second, the posterior distribution of the simulator and the error model parameters $f(\theta, \psi | y_o, x)$ is calculated with the prior distribution $f(\theta, \psi)$ and the likelihood function according to Bayes' theorem:

$$f(\theta, \psi | y_o, x) \propto f(\theta, \psi) f(y_o | \theta, \psi, x) \quad (14)$$

Numerically, properties of the posterior distribution can be approximated based on a sample drawn using a Metropolis-Hastings Markov Chain Monte Carlo (MCMC) algorithm. Details are given in Sect. 3.2.

2.2.3 Predictions in the calibration layout L_1

Third, one has to compute posterior predictive distributions for the observations that have been used for parameter estimation. The experimental layout of this data set (here: calibration layout), L_1 , specifies which output variables are observed, where and when. Here, the model output at calibration layout L_1 is given by the vector $\mathbf{y}^{L_1} = (y_{t_1}^s, \dots, y_{t_{n_1}}^s)$, where y^s denotes the discharge at the location, s , of the measurements and t_j , for $j = 1, \dots, n_1$, the time points of the measurements.

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In order to separate different uncertainty components, we compute predictions from (i) the simulator $\mathbf{y}_M^{L_1}$, which only contains uncertainty from hydrological model parameters, (ii) our best knowledge about the system response $g^{-1}(\tilde{\mathbf{y}}_M^{L_1} + \mathbf{B}_M^{L_1})$, which comprehends additional uncertainty from input errors and structural deficits, and (iii) observations of the system response, $g^{-1}(\tilde{\mathbf{y}}_M^{L_1} + \mathbf{B}_M^{L_1} + \mathbf{E}^{L_1})$ which, in addition, includes random flow measurement errors (note that we mean here the application of the scalar function g^{-1} to all components of the vector specified as its argument). Usually, hydrological “predictions” describe simulation results for time points or locations where we do not have measurements. Here, consistent with Reichert and Schuwirth (2012) and Higdon et al. (2005), “predictions” designate the generation of model outputs (with uncertainty bounds) in general.

To obtain probabilistic predictions for multivariate normal distributions involved in the evaluation of these random variables, the reader is referred to Kollo and von Rosen (2005) and Kendall et al. (1994). Taking as an example the posterior knowledge of the true system output without observation error conditional on model parameters, the expected transformed values are given by

$$E[\tilde{\mathbf{y}}_M^{L_1} + \mathbf{B}_M^{L_1} | \tilde{\mathbf{Y}}_O^{L_1}, \boldsymbol{\theta}, \boldsymbol{\psi}] = \tilde{\mathbf{y}}_M^{L_1} + \boldsymbol{\Sigma}_{B_M^{L_1}} (\boldsymbol{\Sigma}_{E^{L_1}} + \boldsymbol{\Sigma}_{B_M^{L_1}})^{-1} \cdot (\tilde{\mathbf{y}}_O^{L_1} - \tilde{\mathbf{y}}_M^{L_1}) \quad (15)$$

and their covariance matrix by

$$\text{Var}[\tilde{\mathbf{y}}_M^{L_1} + \mathbf{B}_M^{L_1} | \tilde{\mathbf{Y}}_O^{L_1}, \boldsymbol{\theta}, \boldsymbol{\psi}] = \boldsymbol{\Sigma}_{B_M^{L_1}} (\boldsymbol{\Sigma}_{E^{L_1}} + \boldsymbol{\Sigma}_{B_M^{L_1}})^{-1} \boldsymbol{\Sigma}_{E^{L_1}} \quad (16)$$

These equations are used to draw realizations from the bias-corrected output by propagating a large sample from the posterior distribution through the simulator $\mathbf{y}_M^{L_1}$, drawing realizations of $\tilde{\mathbf{y}}_M^{L_1} + \mathbf{B}_M^{L_1}$ and $\tilde{\mathbf{y}}_M^{L_1} + \mathbf{B}_M^{L_1} + \mathbf{E}^{L_1}$ for each point of the sample, and transforming these results back to the original observation scale by applying the inverse transformation g^{-1} . This leads to a sample that approximates the full posterior predictive distribution. To visualize the best knowledge and uncertainty intervals of marginals

of this distribution, it is usually recommendable to compute sample quantile intervals of the individual components (e.g., 0.025, 0.5, 0.975 quantiles).

Besides calculating the posterior predictive distribution, it is important to check the assumptions of the likelihood function. As our posterior represents our knowledge of system outcomes, bias and observation errors, of which not all have a frequentist interpretation, we cannot apply a frequentist test to the residuals of the deterministic model at the best guess of the model parameters. Instead, we have to extract our knowledge of the observation errors to perform a frequentist test. This makes it necessary to split the residuals into bias and observation errors and to derive the posterior of the observation errors alone. A numerical sample of this posterior can be gained by substituting the sample for the random variable $\tilde{\mathbf{y}}_M^{L_1} + \mathbf{B}_M^{L_1}$ in

$$\mathbf{E}^{L_1} = \tilde{\mathbf{y}}_O^{L_1} - (\tilde{\mathbf{y}}_M^{L_1}(\mathbf{x}, \boldsymbol{\theta}) + \mathbf{B}_M^{L_1}). \quad (17)$$

In this equation $\tilde{\mathbf{y}}_O^{L_1}$ refers to the field data. The medians of the components of this sample represent our best point estimates of observation errors that we will use to test the statistical assumptions as described in Sect. 2.2.5.

2.2.4 Predictions in the validation layout L_2

Fourth, one computes posterior predictive distributions for the validation (or extrapolation) layout, L_2 , where data are not available or not used for calibration. In our study, L_2 denotes the location and the time points of the extrapolation range, and the associated model output is given by $\mathbf{y}^{L_2} = (y_{t_{n_1+1}}^S, \dots, y_{t_{n_2}}^S)$.

A sample for layout L_2 could be calculated similarly to the one for L_1 by using the Eqs. (35) and (36) of Reichert and Schuwirth (2012) instead of the Eqs. (15) and (16). However, the specific form of our bias formulation as an Ornstein-Uhlenbeck process (Eqs. 5 and 7) offers a computationally more efficient alternative. As the OU process is a Gauss-Markov process, we can draw a realization iteratively by drawing the realization for the next time step at time t_j from that of the previous time step at time t_{j-1}

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from a normal distribution. The expected value and variance of the normal distribution of the bias given the model parameters is given by

$$E \left[B_{M,j}^{L_2} \mid B_{M,j-1}^{L_2} = b_{j-1}, \boldsymbol{\theta}, \boldsymbol{\psi} \right] = b_{j-1} \cdot \exp \left(-\frac{\Delta t}{\tau} \right), \quad (18)$$

$$\text{Var} \left[B_{M,j}^{L_2} \mid B_{M,j-1}^{L_2}, \boldsymbol{\theta}, \boldsymbol{\psi} \right] = \left(\sigma_{B_{ct}}^2 + (\kappa X_{j-d})^2 \right) \cdot \left(1 - \exp \left(-2\frac{\Delta t}{\tau} \right) \right). \quad (19)$$

The sample of the bias for L_2 can be generated by drawing iteratively from these distributions for all required values of j starting from the last result of each sample point from layout L_1 . By calculating the results of the deterministic model and drawing from the observation error distribution, samples for $\mathbf{y}_M^{L_2}$, $g^{-1}(\tilde{\mathbf{y}}_M^{L_2} + \mathbf{B}_M^{L_2})$, and $g^{-1}(\tilde{\mathbf{y}}_M^{L_2} + \mathbf{B}_M^{L_2} + \mathbf{E}^{L_2})$ can be constructed similarly as for the layout L_1 .

2.2.5 Performance analysis

Fifth, the quality of the predictions is evaluated by assessing (i) the coverage of prediction for the validation layout and (ii) whether the statistical assumptions underlying the error model are met for the calibration layout.

15 Checking the predictive capabilities

The predictive capability of the model can be assessed by two metrics, the “reliability” and the “sharpness” (Breinholt et al., 2012). The reliability measures what percentage of the validation data are included in the 95 % credibility intervals of $g^{-1}(\tilde{\mathbf{y}}_M + \mathbf{B}_M + \mathbf{E})$. When this percentage is larger than or equal to 95 %, the predictions are reliable. Note that in general we expect this percentage to be larger than 95 % as our uncertainty bands describe our knowledge about future predictions. This combines lack of knowledge of parameter values and bias with the uncertainty due to the observation error

and thus is systematically more uncertain than the observation error alone. The limiting case of an exact coverage is only expected to occur if parameter uncertainty and bias is small compared to the observation error. In contrast, the sharpness measures the average width of the 95 % credibility intervals. Ideally, we seek the narrowest reliable bands. Besides these two criteria, the Nash–Sutcliffe efficiency index (Nash and Sutcliffe, 1970) is used to evaluate goodness of fit of the deterministic model to the data.

As a side note, it has been suggested to check the prediction performance of a model by only examining the number of data points included in the prediction uncertainty intervals resulting only from parameter uncertainty (Dotto et al., 2011). Unfortunately, this is not conclusive because the field observations are not realizations of the deterministic model but of the model plus the errors.

Checking the underlying statistical assumptions

The underlying statistical assumption of the error model is usually verified by residual analysis. This, however, is only meaningful for frequentist quantities. In a Bayesian framework, probabilities express beliefs, which can differ from one data analyst to another and thus cannot be tested. In our error model (Eq. 4), the observation error is the frequentist part of the likelihood function and frequentist tests can thus only be applied to this term. As outlined in Sect. 2.2.3, we can use the median of the posterior of the observation error at layout L_1 to do such a frequentist test. These posterior observation errors should be tested whether they are (i) normally distributed, (ii) have constant variance and (iii) are not autocorrelated. As the observation errors may only represent a small share of the residuals of the deterministic model, posterior predictive analysis based on independent data, as outlined in the previous paragraph, remains an important performance measure.

As a side note, it is conceptually incorrect to check frequentist assumptions by using the full (Bayesian) posterior distribution (e.g., Renard et al., 2010). Using the full posterior instead of the best point estimate of the observation errors adds additional

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uncertainty from the incomplete prior knowledge of parameter values. In our view, this distorts the interpretation of frequentist tests.

2.2.6 Improving the simulator

Finally, after performance checking, one should evaluate the opportunity to improve the simulator and/or the measurement design for the model's input. Hints for improvement can be obtained by exploratory analysis of the bias, for example by investigating the relation between its median and output variables or input. On the one hand, systematic patterns in the relation of the bias to model input or output would suggest the presence of model structural deficits that could be corrected. On the other hand, increasing variance of the bias with increasing discharge could be a sign of excessive uncertainty in rainfall data. This could be improved by more reliable rainfall information.

3 Material

To demonstrate the applicability and usefulness of our approach, we evaluate the performance of nine different error models in a real-world urban drainage modeling study. In the following we will briefly describe the case study and details on the numerical implementation of the bias framework.

3.1 Case study

We tested the uncertainty analysis techniques on a small urban catchment in Sadová, Hostivice in the vicinity of Prague (CZ). The system has an area of 11.2 ha and is drained by a separate sewer system. It is a residential area with an "Open Housing" land-use type and has an average slope of circa 2 %.

The monitoring data of rainfall and runoff were collected in summer 2010 (Bareš et al., 2010). Flow was measured at the outlet of the stormwater system in a circular PVC pipe with a diameter of 0.6 m. A PCM Nivus area-velocity flow meter was used

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to record water level and mean velocity every 2 min. These output data show that the hydrosystem is extremely dynamic, with a response ranging approximately from 2 L s^{-1} during dry weather to 600 L s^{-1} during strong rainfall.

Rainfall intensities were measured with two tipping bucket rain gauges that were installed only a few hundred meters from the catchment (Fig. 2). These two input temporal datasets have been aggregated to 2 min time steps based on the weighted average distance from the watershed centroid.

For model calibration, we selected two periods with 6 major rainfall events. One on 27 August between 01:52 LT and 12:58, and the second in July between 22 July at 23:32 and 23 July at 19:00. For validation, a single period from 23 July at 19:02 to the next day at 07:00 was selected. The calibration and validation data of July 2010 are illustrated in Fig. 5.

3.2 Model implementation

We modelled runoff in the stormwater system using the SWMM software (Rossman and Supply, 2010). The model was set to a simple configuration, namely a nonlinear reservoir representing the catchment connected to a pipe with a constant groundwater inflow. Lumped modeling is particularly appropriate when a study focuses on outlet discharge and computation can be a limiting factor (Coutu et al., 2012). The parameters that we inferred during calibration were the imperviousness, the width, the dry weather inflow, the length of the conduit and the slope of the catchment.

The procedure outlined in Sect. 2.2 to compute the posterior predictive distributions was implemented in R (R Development Core Team). SWMM was called from R using the `shell` command. For a simulation, an input file with parameters and rainfall series was read and the modelled stormwater discharge was written to an output file. The input file was iteratively modified to update the parameters by using `awk` (Aho et al., 1987). `awk` was also used to extract the runoff time series from the output file.

From a numerical viewpoint, we solved the “inverse problem” described in Sect. 2.2.2 by using a Metropolis-Hastings Markov Chain Monte Carlo (MCMC) algorithm

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(Hastings, 1970). Before sampling from $f(\theta, \psi | y_o, x)$, we obtained a suitable jump distribution (a.k.a. transition function or proposal density) by using a stochastic adaptive technique to draw from the posterior (Haario et al., 2001). For better performance we added a size-scaling step, which depends on the target acceptance rate. For our inference problem, this algorithm proved to be more robust than others, such as Vihola (2012) and Haario et al. (2006). However, research on efficient techniques for posterior sampling is evolving rapidly and other approaches could also be used. See Liang et al. (2011) and Laloy and Vrugt (2012) for recent developments in Bayesian computation.

4 Results

In general, accounting for model bias produced substantially more reliable predictions than using simple error models. Simulations using simplistic error models generally met the statistical assumptions much less, independent of the transformations applied. In the following, we will first give details on the predictive performances of the different error models and then show what can be learned from the distribution of the estimated observation errors.

4.1 Evaluating the performance of probabilistic sewer flow predictions

As expected, the different assumptions underlying the nine error models lead to different credibility intervals for stormwater runoff at the monitoring point (Fig. 4 and Table 1). Predictions did not exhibit considerable sensitivity to the prior for the bias (results not shown).

For our case study, the best error model clearly was the constant bias model with log-sinh transformation (Fig. 5). It has a high reliability, sharpness and Nash-Sutcliffe index. The worst error model was the iid with log-sinh transformation, which performed very poorly in the extrapolation range, with less than 50 % validation data included in the total uncertainty bands.

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Although the deterministic model reproduced the measured discharge dynamics well, the total uncertainty during strong rain events in the validation period is still rather large. Indeed, as illustrated in Fig. 5, even the best performing error model has a 95 % interquartile range up to $\sim 140 \text{ L s}^{-1}$, which is about 20 % of the maximum runoff modeled in the extrapolation phase.

In general, we found that most of the error formulations with model bias produced reliable predictions and around 95 % or more of validation data fell within the 95 % prediction interval range for new observations (Table 1). In addition, the bias framework successfully separated the total uncertainty into parametric uncertainty, effect of input plus structural deficits, and observation errors (Figs. 4 and 5). All the autoregressive error models indicated that most of the predictive uncertainty is due to model bias. Interestingly, uncertainty due to random measurement noise is generally so small that it is not visible in the plots.

In contrast, all error models which ignore model bias generated overconfident predictions with too narrow uncertainty bands. This was almost independent of the transformation applied. As stated above, they also could not separate the total uncertainty since input and structural errors were implicitly assumed to be non-existent and thus did not give any information on the importance of the individual error contributions.

Besides providing reliable estimates of the total predictive uncertainty, a second advantage of the bias framework is that it takes into account the different knowledge about the calibration and validation layout. As shown in Fig. 4, the predictions obtained with bias description for the calibration layout, to the left of the dotted line, included most of the observations while being, at the same time, very narrow. This takes into account that in the calibration range, where data are available, our knowledge on stormwater runoff is rather accurate and precise. In contrast, for the extrapolation domain where no observations are available, the uncertainty intervals are much larger.

In addition, we found that the conditioning on the monitoring data become increasingly the further the model predicts into the future. This gradually increases the uncertainty in the transition phase as the prediction horizon moves from the past into the

future. Again, this is not possible with the traditional error models. As they cannot distinguish between past and future information, their prediction intervals are equally wide for both the calibration and validation layouts.

A third advantage of bias description is that it provides an estimate of the most probable system response $g^{-1}(\tilde{y}_M + \mathbf{B}_M)$, which is depicted by the dashed line in Fig. 4. In the calibration layout, it closely follows the observations, which are comparably precise and therefore contain the best information on the state of the system. For the validation layout, this information is lacking. However, instead of abruptly reverting to the simulator, the transition is gradual because the autocorrelated bias carries the information from the last monitoring data into the future. We found that the de-correlation typically takes a few correlation lengths (here circa 30–50 min).

As can be seen in Table 1 and Fig. 4, even though the uncertainty intervals are more reliable when bias is considered, the deterministic model performs best when residual autocorrelation and heteroscedasticity are not taken into account. This is not surprising since maximizing the posterior with the simple iid error model with no transformation corresponds to minimizing the sum of the squares of the errors and therefore produces the best fit.

Comparing the input-independent and dependent bias formulations, two important points are observed. First, the constant bias description produced on average “sharper” uncertainty bands than the input-dependent version. The latter, in particular, produced huge uncertainties during rain events and very narrow intervals during dry weather. Second, as expressed in Table 1, the constant bias almost produced the same simulator fit as the simple error model, whereas the input-dependent bias formulation performed less satisfactorily.

The transformation created skewed predictive distributions and, as expected, increased the wet weather uncertainty in the “real” space. This substantially reduced occurrence of negative predicted flows with the Box-Cox transformation, and avoided them altogether with log-sinh. The most noticeable observation about transformation is that combining the input-dependent bias with the Box-Cox transformation we

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obtained the largest uncertainty bands and among the poorest deterministic model performances.

4.2 Analysis of estimated observation errors

In general, the analysis of the measurement errors is consistent with the predictive performance analysis. Again, the error model with a constant bias and the log-sinh transformation best fulfills the statistical assumptions (Fig. 6). The frequentist component of the residuals (the estimate of the observation errors) is virtually normally distributed, has an almost constant variance and no autocorrelation. Diagnostic plots on E are only shown as “Supplement” since the magnitude of these errors, which are extremely small compared to the bias, suggests that the usefulness of formal statistical tests can be questioned in this case.

In contrast, the residuals of the iid error models are heteroskedastic and heavily autocorrelated and thus strongly violate the statistical assumptions. They are also several orders of magnitude larger than those with bias description. Such huge residuals clearly lose their interpretative significance as random measurement errors of the flow.

Finally, besides frequentist analyses of the white measurement noise, one should check what can be learned from an exploratory analysis of the model bias. Plotting the model bias against flow data (Fig. 3) shows an almost constant scatter with only weak trends. In general, we observed a negative bias in the intermediate flow range and a positive bias during severe storms. While the first systematic deviation is caused by slightly overestimating the runoff in the decreasing limb of the hydrograph, the second reveals that the model systematically underestimates the highest peak discharges (see Fig. 5).

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5 Discussion

The outcomes of this study, in agreement with theoretical considerations, confirmed that describing bias by means of a stochastic process produces much more reliable and interpretable hydrological predictions than the overly-simplistic traditional error model.

5 Additionally, the bias error model naturally describes the increase in uncertainty of the system response when passing from the calibration to the extrapolation range. In the following, we will interpret the results obtained for our system, assess the differences among the proposed bias description formulations, analyze the dissimilarities between natural and urban hydrology, and finally provide guidelines on how to describe model
10 discrepancies in future studies.

5.1 Bias analysis in the case study

The analysis of the uncertainties in our stormwater system demonstrated that our parsimonious deterministic model captures most of the hydrograph dynamics. Nevertheless, it produced partially biased simulations. By accounting for these systematic deviations
15 with the most plausible error model, we observed almost a constant variance of the estimated observation errors. Furthermore, this configuration displayed some negative bias during intermediate rain events and positive bias with very high discharges. These findings indicate that a part of the predictive uncertainty stems from imprecise precipitation measurements, which increases the scatter of the residuals. Another part of
20 prediction uncertainty, instead, stems from structural deficits due to oversimplification of the simulator, which produce systematic trends in the residuals.

If the study's goal is to reduce prediction uncertainty, one should, after detecting structural deficiencies, improve the model. This can be done by either selecting other process formulations (see Reichert and Mieleitner, 2009) or increasing the model complexity. In our case, analyzing how model discrepancies depend on the measured discharge
25 gave us the necessary information to improve the simulator. Increasing the

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number of calibration parameters from preliminary simulations reduced a strong positive bias (results not shown) to some mild systematic trends (Fig. 3).

5.2 Comparison of different bias descriptions

In this paper we proposed 5 different descriptions of model inadequacy. The bias description where the variance quadratically increases with precipitation is the conceptually most appealing form since it mechanistically accounts for higher uncertainty during rainy periods. Furthermore, in contrast to the empirical output-dependence via data transformation, input-dependence acknowledges that the rising limb of the hydrograph is more uncertain than the recessive limb.

Notwithstanding its theoretical appeal, the input-dependent bias has several drawbacks. First, it has two parameters more than the constant bias, which potentially reduces the robustness of this approach. In particular, during estimation, the proportionality constant κ tends to reach very high posterior values (see Supplement for priors and posteriors) and, in this way, leads to inflated variances during rainfall and too small variances during dry weather. Second, since we always assume a normal distribution of the bias, the input-dependent description frequently requires a transformation anyway in order to avoid physically meaningless negative uncertainty bands. Third, linked to the two previous considerations, the input and output dependent error model has the tendency to include too many mechanisms to describe model inadequacy. This complex representation reproduces data dynamics “excessively” well and therefore motivates the deterministic model to fit the observations less. Finally, if larger uncertainties during storms are due to structural deficits rather than to erroneous input measurements, a variance increasing with precipitation would be also conceptually suboptimal.

It is interesting to notice that the input-dependent error model never reverted back to a constant bias (i.e. κ never calibrated to 0), even in cases where all performance indicators favored the simpler error description. This can be explained considering that the input-dependent bias has a basic variance plus a variance induced by precipitation. In our case, the posterior basic variance for the input-dependent bias was, irrespective

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of the transformation, smaller than for the constant bias. This is caused by three combined phenomena: (i) an error distribution with smaller variance has generally higher likelihood, (ii) our simulator could match the baseflow almost exactly, and (iii) a large part of the calibration period had an output equal to the baseflow. Since the input-dependent error model still had to account for big errors during wet weather, it did so by increasing the precipitation-induced error variance, producing sometimes too wide uncertainty intervals for the future storm events.

5.3 Bias assessment in urban and natural hydrology

Interestingly, for Honti et al. (2013) the input-dependent Box-Cox transformed error model produced the best predictions. This different outcome, however, is not necessarily in contrast with our findings. First, as mentioned in the introduction, different case studies can display extremely dissimilar error properties. Our urban catchment had a much stronger difference in the hydrologic response between dry and wet periods than Honti et al.'s natural watershed, which additionally presented fewer points of constant minimal discharge. Second, the formulation by Honti et al. (2013) presented an additional precipitation-dependent bias component, while neglecting the delay between precipitation occurrence and uncertainty increase. Thirdly, in Honti et al. (2013) the log-sinh transformation was not implemented, and comparing only the Box-Cox transformed input-dependent and constant bias we also find that the first produces better coverage of the validation data.

Comparing urban to natural catchments, an important aspect is, first, that urban hydrosystems react much more rapidly and strongly and therefore require much more frequent measurements of the hydrologic response (typically at minute scale instead of daily scale). Furthermore, the discharge in sewers can be ascertained with much higher precision and accuracy than in the case of rivers. Indeed, in drainage conduits the area-velocity sensors can measure the velocity directly, without requiring a rating curve, which is an additional source of uncertainty in streamflow observations (Sikorska et al., 2013; Montanari and Di Baldassarre, 2013). The elevated temporal density and

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precision of the measurements, as discussed by Reichert and Mieleitner (2009), leads to an even higher need to address model discrepancies explicitly.

Second, in natural watersheds the high flow can be associated with floodplain inundations which dramatically increase the uncertainty of flow measurements. In sewer systems, by contrast, the well defined geometry of the pipes and the reliable flow measurement devices lead to a much smaller increase in observation uncertainty with increasing discharge. This situation underlines the advantage of a log-sinh transformation in urban hydrology instead of the traditional Box-Cox. Indeed, the former assumes that residual scatter in high streamflow ranges is limited.

Regarding uncertainty estimation, it seems that a formulation where the standard deviation of the input-dependent bias component linearly increases with precipitation is suboptimal for urban systems. Indeed, most urban water basins, especially those only draining stormwater and having low groundwater infiltration, exhibit extremely high contrasts between low and high flows. With such a strong dynamism and linear input dependence, unnecessarily wide uncertainty intervals can be produced.

5.4 Recommendations

As our results demonstrate, model deficiencies have to be considered in hydrological predictions, especially when dealing with urbanized areas. This is in agreement with many other studies (Breinholt et al., 2012; Yang et al., 2007b; Schoups and Vrugt, 2010; Reichert and Mieleitner, 2009). If the modeller is not interested in separating predictive uncertainty into its contributing sources because data collection or model building processes are fixed, we suggest using a lumped autoregressive error model (Bates and Campbell, 2001; Yang et al., 2007b; Schoups and Vrugt, 2010). Such formulations are usually sufficient to reliably estimate total output uncertainty. However, it is often useful to assess how far the prediction uncertainty can be reduced by minimizing a particular error source (Sikorska et al., 2012). In these cases, we recommend applying our five-variant bias description in order to disentangle the effects of model discrepancies and random measurement errors. In particular, we suggest starting with

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a constant log-sinh transformed bias and setting priors of the error model parameters using the recommendations given in Sect. 2.2.1. This likelihood formulation is simple and robust and proved to perform extremely well in our case study. Then, if the efficiency of this error description is unsatisfactory, the Box-Cox transformation and eventually the input-dependent bias description in its three variants can be applied. Finally, we propose selecting among the error description providing the best validation coverage with the narrowest bands and the most iid transformed observation errors, and applying this likelihood formulation to subsequent predictions.

If the input-dependence is of particular interest though providing dubious predictions, considering what we discussed above, we suggest adapting this dependence on precipitation as a function of the systems dynamics. One possibility could be to modify Eq. (7) and, instead of a linear increase of uncertainty with the precipitation, one could adopt a power relationship with the exponent as calibration parameter.

6 Conclusions

In this study, we investigated different strategies for describing systematic errors in hydrological modeling. Although this methodology was primarily developed for urban drainage studies, it is not only statistically sound, but also flexible. Therefore it is very suitable for analyzing other similar input-driven systems such as natural catchments. Our objective was, first, to obtain reliable flow predictions that take into account model bias. Second, we set out to quantify the different error contributions. We adapted the Bayesian description of model discrepancy suggested by Craig et al. (2001); Kennedy and O'Hagan (2001); Higdon et al. (2005); Bayarri et al. (2007); Reichert and Schuwirth (2012) to urban hydrology, making the bias variance increase during wet weather in five different ways. The best results were obtained by making the variance output-dependent, specifically with a bias having a constant variance in a log-sinh transformed space. This consideration is based on residual analysis in the calibration period and the coverage and width of the prediction intervals in the validation phase. From the

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experience gained in this modeling study and theoretical considerations, we conclude that:

- i. Due to input uncertainty, structural deficits, and (possibly) systematic errors in flow measurements, urban hydrological simulations are biased. When using precise and high-frequency output measurements to calibrate and analyze the uncertainties of these simulators by means of traditional iid error models, we obtain implausible predictions.
- ii. We can obtain much sounder predictions and significantly improve the fulfillment of the assumptions by adding a model discrepancy function to the classical error model. Such a bias term should have a variance that increases during storm events as a function of rainfall and/or runoff. Finally, the results demonstrate that random output observation errors are much smaller than uncertainty due to bias.
- iii. In our study, a rather simple constant autoregressive bias with a log-sinh transformation outperformed an input-dependent bias description. Although the latter is conceptually superior, the simpler formulation appeared more suitable for systems with alternating long low flow periods and short high discharge pulses, as happens with urban drainage basins. Indeed, it is apparently less susceptible to producing excessively wide error bands and suboptimal fit. Therefore it is the first one that we suggest applying for urban hydrological uncertainty analysis, followed by the other four recommended variants.
- iv. Although it generally outperforms the traditional error assumptions, we are aware of the limitations of our approach. The presence of bias, to which we have to assign a weight in the form of priors, inevitably introduces subjectivity in the uncertainty analysis. Moreover, this statistical method can “only” describe the different types of output uncertainties, but cannot address directly the causes of bias nor can it straightforwardly lead to an uncertainty reduction.

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- v. Despite remaining challenges, our approach has further advantages besides providing separated and credible prediction intervals. First, a bias description can be associated with a fully fledged uncertainty propagation framework, supporting bias reduction, to describe “remnant” errors. So far, this remaining bias due to imperfect description of the uncertainty sources has been modeled as white noise. Second, the exploratory analysis of model bias, for example investigating its dependence on the output, can provide valuable insight into whether it is dominated by input uncertainty or inadequate model formulation. Third, this statistically sound approach is computationally not more intensive than the classical methods. It is even much cheaper than the mechanistic error propagation frameworks.
- vi. Open questions requiring further research include establishing how the bias description can be applied to quantify the structural errors of complex hydrodynamic models with multiple outputs. Moreover, it is unclear how input errors can be separated from structural deficits as this requires a probabilistic formulation and propagation through the simulator. A further challenge is that complex sewer models are prohibitively slow for many iterative simulations. This can be possibly overcome by statistical approximations, such as emulators.

Supplementary material related to this article is available online at:

[http://www.hydrol-earth-syst-sci-discuss.net/10/5121/2013/](http://www.hydrol-earth-syst-sci-discuss.net/10/5121/2013/hessd-10-5121-2013-supplement.pdf)

[hessd-10-5121-2013-supplement.pdf](http://www.hydrol-earth-syst-sci-discuss.net/10/5121/2013/hessd-10-5121-2013-supplement.pdf)

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Table 1. Prediction performance metrics for the different error models: iid untransformed error model (iidE), Box-Cox transformed (iidE.BC), and log-sinh transformed (iidE.ls), constant untransformed bias (CtB), Box-Cox transformed (CtB.BC), and log-sinh transformed (CtB.ls), input-dependent untransformed bias (IDB), Box-Cox transformed (IDB.BC), and log-sinh transformed (IDB.ls). The criteria on the left represent the Nash-Sutcliffe index in calibration (NS.cal) and validation (NS.val) phases in the non-transformed space, the percentage of validation data points falling into 95 % prediction interval (Cover.val), and the bounds average width [$L s^{-1}$] in the extrapolation domain (Sharp.val).

	iidE	iidE.BC	iidE.ls	CtB	CtB.BC	CtB.ls	IDB	IDB.BC	IDB.ls
NS.cal	0.947	0.924	0.921	0.897	0.921	0.872	0.855	0.824	0.809
NS.val	0.838	0.783	0.764	0.84	0.829	0.815	0.732	0.73	0.696
Cover.val	86.9	62.2	44.2	93.9	79.7	97.8	93.6	99.4	75
Sharp.val	40.3	22.6	18.7	66.9	27.9	54.1	76.1	179	60.5

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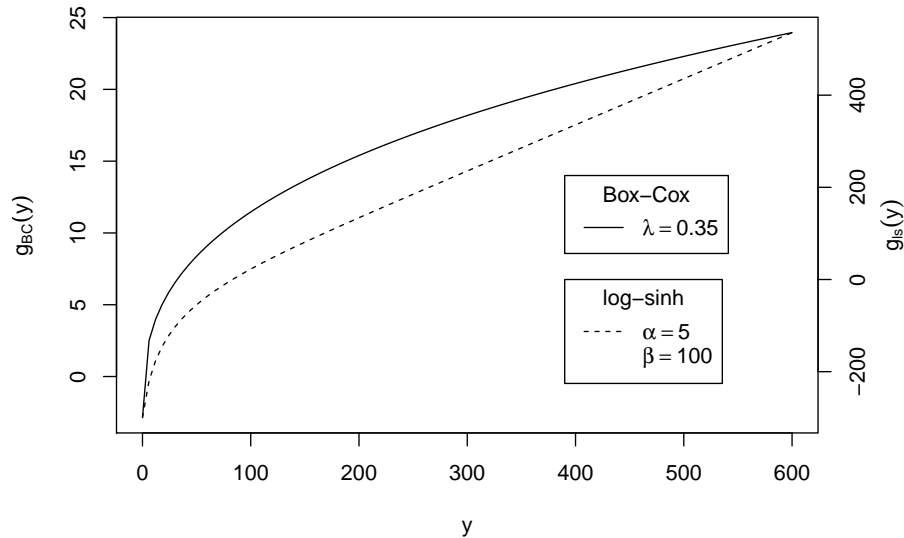



Fig. 1. Behavior of the Box-Cox (solid line) and log-sinh (dashed line) transformation as a function of the output variable (e.g. discharge in $L s^{-1}$) with parameters used in this study.

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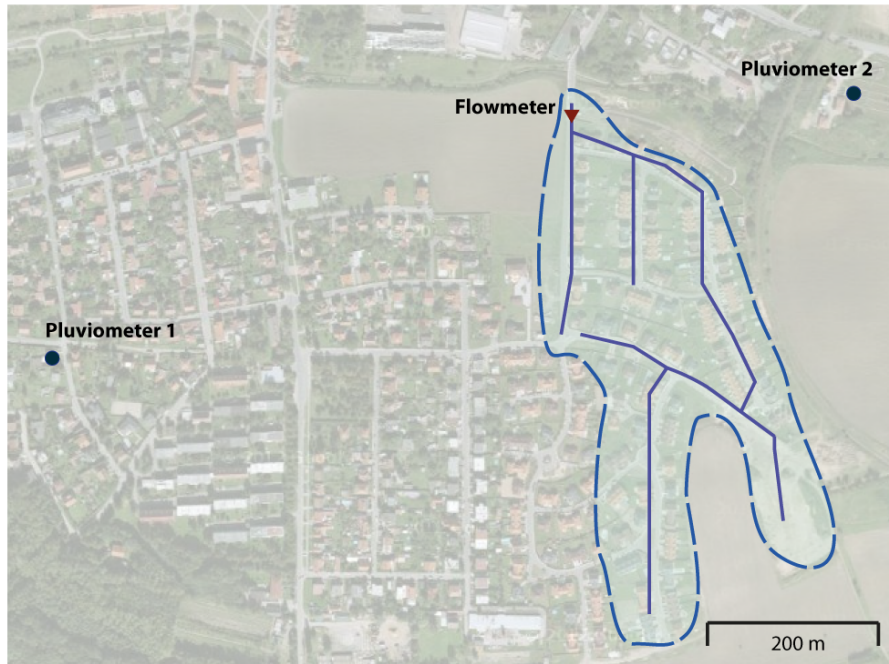


Fig. 2. Aerial photo of our Sadová case study catchment. The map shows the layout of the main stormwater conduits and the location of the rain gauges and the flow meter.

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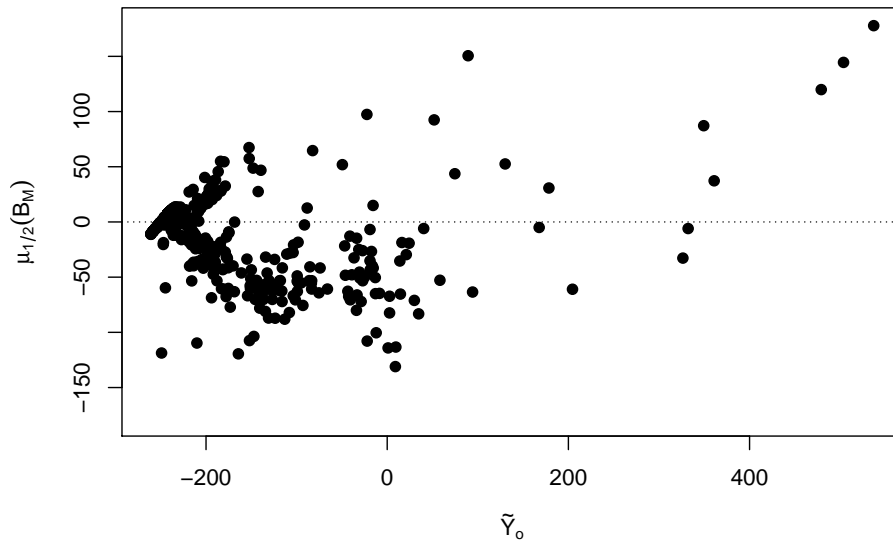


Fig. 3. Median of model inadequacy versus transformed observed runoff for the calibration period shown in Fig. 5. Results are shown for the best solution: the constant bias log-sinh transformed error model.

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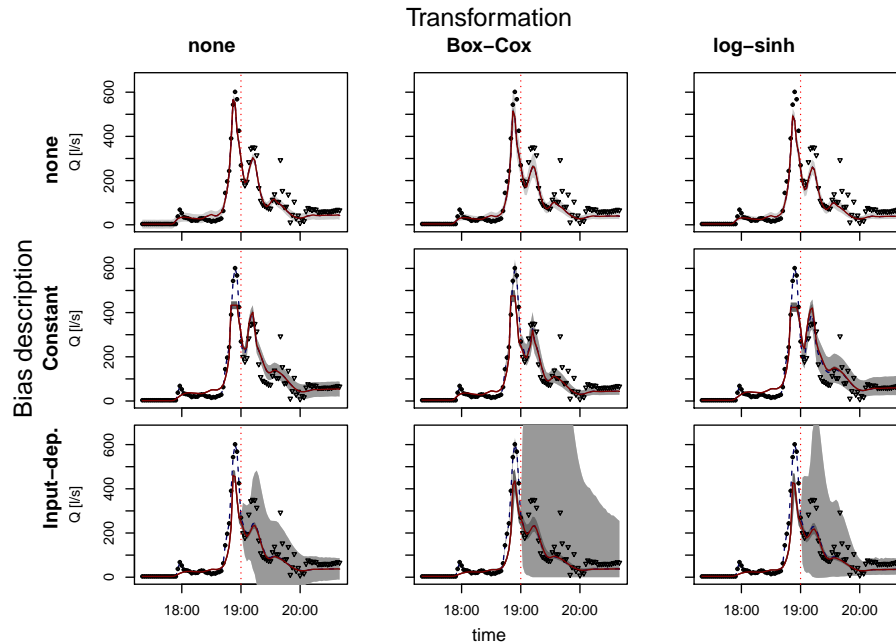


Fig. 4. 95 % credible intervals for flow predictions for transition phase obtained with different assumptions on error distribution. The vertical dashed line divides the calibration layout (past) from the validation layout (future). The solid line is the deterministic model output with the optimized parameter set, whereas the dashed line is the bias-corrected output representing our best estimation of the true system response. Observed output of the system is represented by dots, with the triangular ones not being used for calibration. Colors of the credibility intervals: deterministic model predictions (dark gray), predictions of the real system output (intermediate gray), predictions of new observations (light gray). The observation errors, being very small for this scale ($< 1 \text{ L s}^{-1}$), the last two uncertainty bands overlap and only the intermediate gray is visible.

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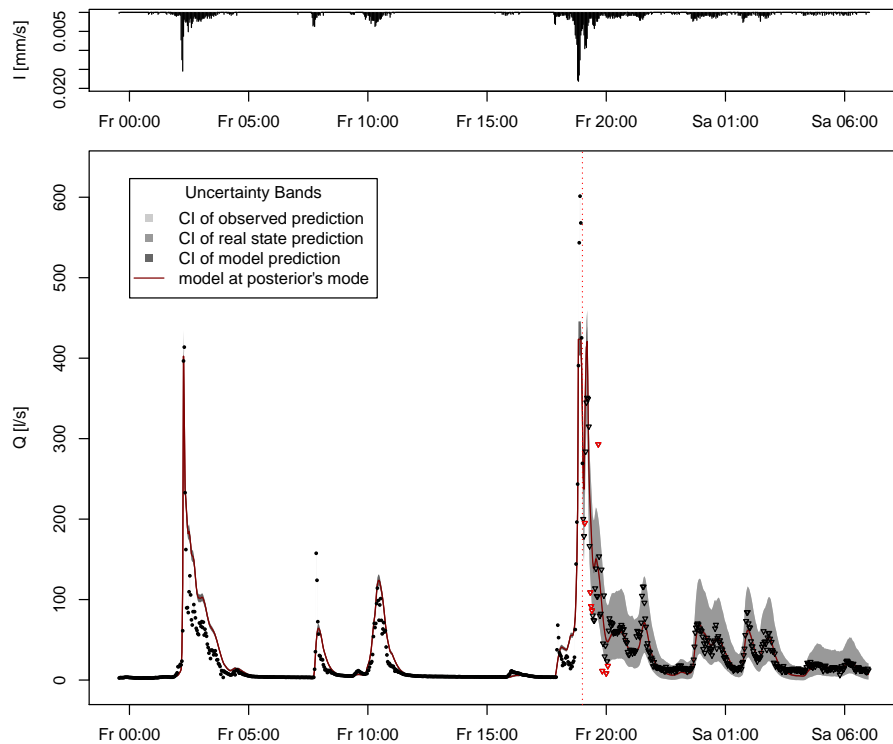


Fig. 5. Probabilistic runoff predictions for part of the calibration (left) and the full validation period (right) with the constant bias log-sinh transformed error model. The input time series is shown on the top. Color and symbol interpretation is the same as in Fig. 4. Additionally, validation data not included in 95 % credible intervals of new observations are marked in red.

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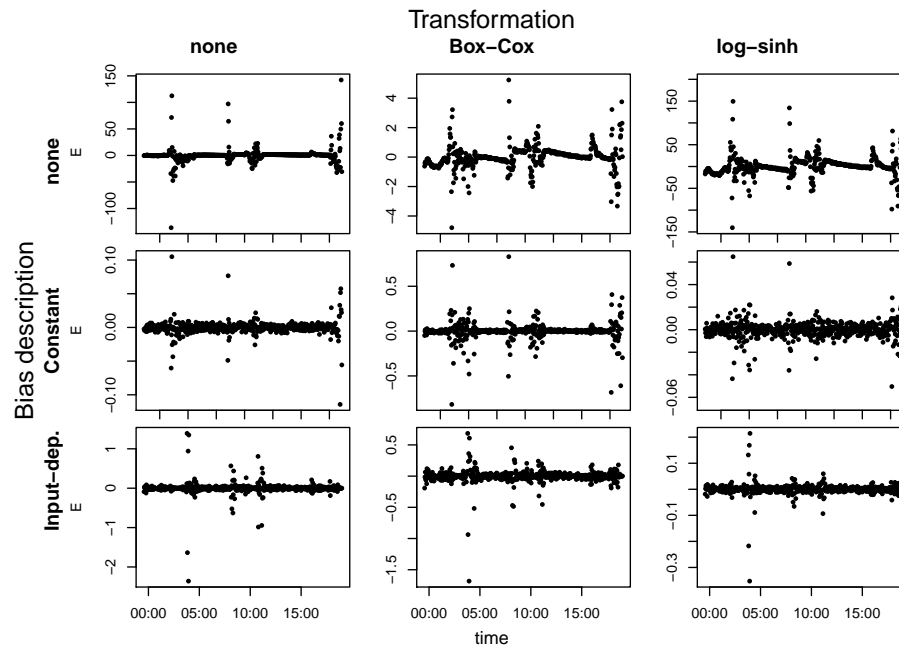


Fig. 6. Time series of median of E , the part of residuals assumed to come from random observation errors. The range illustrated is the same part of the calibration period as shown in Fig. 5. The ordinate axis is in transformed flow units.

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