International Environmental Modelling and Software Society (iEMSs)
2012 International Congress on Environmental Modelling and Software
Managing Resources of a Limited Planet, Sixth Biennial Meeting, Leipzig, Germany
R. Seppelt, A.A. Voinov, S. Lange, D. Bankamp (Eds.)
http://www.iemss.org/society/index.php/iemss-2012-proceedings

Relative importance of secondary settling tank models in WWTP simulations – A global sensitivity analysis using BSM2

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Abstract: Results obtained in a study using the Benchmark Simulation Model No. 1 (BSM1) show that a one-dimensional secondary settling tank (1-D SST) model structure and its parameters are among the most significant sources of uncertainty in wastewater treatment plant (WWTP) simulations [Ramin et al., 2011]. The sensitivity results consistently indicate that the prediction of sludge production is most sensitive to the variation of the settling parameters. In the present study, we use the Benchmark Simulation Model No. 2 (BSM2), a plant-wide benchmark, that combines the Activated Sludge Model No. 1 (ASM1) with the Anaerobic Digestion Model No. 1 (ADM1). We use BSM2 as a vehicle to compare two different 1-D SST models, and to assess the relative significance of their performance on WWTP simulation model outputs. The two 1-D SST models assessed include the first-order model by Takács et al. [1991] and the second-order convection-dispersion tool [Plósz et al., 2007]. Additionally, we assess the impact of two operational strategies for excess activated sludge wastage on simulation performance. A global sensitivity analysis (GSA) on BSM2 was carried out using two methods: (a) linear regression of Monte Carlo simulations (SRC method); and (b) Morris screening. The overall objective of assessing the 1-D SST model selection and parameters in GSA is to provide a parameter sensitivity ranking for WWTP calibration exercises, aiming at predicting key plant performance criteria, including methane production and effluent water quality index. Results obtained in this study show that, 1-D SST model parameters strongly influence biogas production via anaerobic digestion and the plant's effluent water quality, but they have limited effect on estimating the quality of nitrogen rich returns from the digester.

***Keywords**:* Modelling; ASM; BSM; water quality; simulators; uncertainty; good m-odelling practice; sensitivity analysis

1 INTRODUCTION

Depending on the engineering objective, assessing the sensitivity of the selected model outputs to model parameters can help practitioners optimize the model calibration task. For wastewater engineering, the secondary settling tank (SST) model selection and calibration are not trivial exercises, and require a stepwise systematic approach – e.g., the one proposed by Ramin and Plósz [2012], shown in Fig. 1. Engineering objectives, requiring some form of SST modelling, comprise SST design (preliminary, detailed assessment), SST trouble-shooting, sizing bioreactors combined with SST, wastewater treatment plant (WWTP) modelling and decision support and WWTP control.

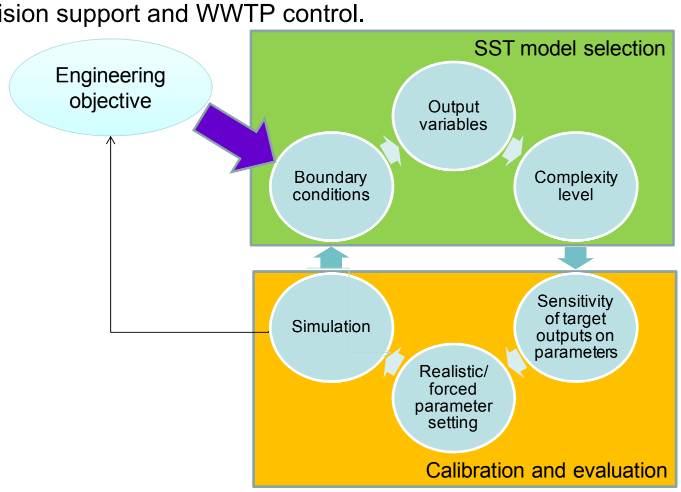

Figure 1. Layout of a typical exercise of model selection and calibration/evaluation for secondary settling tank (SST) simulation [Ramin and Plósz, 2012].

Firstly, once the engineering objective is defined, practitioners should define the boundary conditions of the SST system in terms of design (simple: surface and depth of SST, versus detailed: also the inner structure of SST and sludge collection mechanism), flow-rate conditions (constant, dry weather, dry- and wet weather), settling characteristics (optimum and/or bulking/pin-point). Secondly, the SST model output variables should be selected for the given engineering task, including, for example for one-dimensional (1-D) models, the effluent total suspended solid (TSS) concentration ($X_{TSS,Eff}$), TSS concentration in the return activated sludge (RAS) stream ($X_{TSS,RAS}$), and the sludge blanket height (SBH). Thirdly, based on the selected boundary conditions and the target output variables requirements of a specific engineering objective, practitioners would select a suitable SST model complexity level. For WWTP models, requiring the simulation of SST in combination with bioreactors, depending on the specific engineering objective, predominantly, zero- or 1-D models are used. This paper focuses on one-dimensional secondary settling tank (1-D SST) simulation models that comprise first-order, 1-D^{1st} (e.g., Takács et al. [1991]) and second-order, 1-D^{2nd} (e.g., Diehl and Jeppsson [1998]; Plósz et al. [2007]; De Clercq et al. [2008]) models. For WWTP models, an International Water Association (IWA) Scientific Technical Report has elaborated on good modelling practice [Rieger et al., 2012], guiding wastewater engineers in model selection and calibration exercises, among others. For plant-wide model calibration and parameter selection global sensitivity analysis (GSA) results can for example be used to prioritize parameters as a function of the set of target variables. In the iterative calibration exercise for plant-wide simulations, for the calibration of a SST model, hindered settling velocity parameters (r_H and v_0) and non-settleable fraction (f_{NS}) parameters can be set either using mostly forced calibration for 1-D^{1st} or using realistic/measured values for 1-D^{2nd} models. By forced calibration we mean the arbitrary manipulation of model parameter values to obtain a desirable SST model output ("fine-tuning"). In theory (see Takács et al. [1991]; Plósz et al. [2011]), for 1-D^{1st}, forced calibration of the SST model should be carried out separately under wet and dry-weather flow conditions. Simulation under wet-weather flow conditions thus requires a different set or multiple sets of parameters, depending on the range of the flow boundaries. For 1-D^{2nd}, including an explicit flow-dependent dispersion coefficient (Watts et al. [1996]; Plósz et al. [2007]; De Clercq et al. [2008]), dry- and wet-weather flow conditions can be modeled using one calibration setting. A precondition of such 1-D^{2nd} calibration is that the calibration of the flow dependent dispersion coefficient should be representative of the range of the flow boundary conditions imposed. As to settling boundary conditions imposed, any 1-D^{1st} model is limited to predict SST performance under non-ideal conditions, e.g., bulking, since measured settling velocity parameters cannot be explicitly represented in the model. This is not the case for 1-D^{2nd} models, which can accommodate measured/realistic settling velocity parameters.

In WWTP simulators, unfortunately, still very few 1-D^{2nd} model implementations exist, and most simulation studies thus use the 1-D^{1st} model of Takács et al. [1991]. In previous assessments, 1-D SST models and settling model parameters were subject to uncertainty analysis in only one global sensitivity assessment [Benedetti et al., 2008] using 1-D^{1st}. In the Benchmark Simulation Model No. 1 (BSM1) [Copp, 2002], default settling model parameters were chosen such that settling poses no real problems to the plant performance [Sin et al., 2011]. A rigorous sensitivity assessment of activated sludge treatment performance to 1-D^{1st} and 1-D^{2nd} parameters was first presented by Ramin and Plósz [2012]. This study, employing the BSM1, demonstrates that 1-D SST models and their parameters are the most significant sources of uncertainties, impacting plant performance criteria, e.g., solids retention time (SRT). Using measured settling parameters in 1-D^{1st} can cause numerous inefficiencies in predicting the activated sludge system performance (e.g., Plósz et al. [2011]). In practice, such shortcomings can drive engineers to selecting simpler zero-D SST models that may be inadequate for the selected engineering objective. The BSM1 and 2 are simulation models, used to evaluate control performance. In comparison, BSM2 (Jeppsson et al. [2007]; Nopens et al. [2010]) includes more realistic influent flow-rate and concentration boundary conditions imposed on the simulation model [Gernaey et al., 2011], comprising the activated sludge process in combination with anaerobic sludge digestion.

In the present global sensitivity analysis (GSA) study, we applied two methods: (i) the linear regression of Monte Carlo simulations (SRCs method); and (ii) Morris Screening. The SRCs method is performed in most of the GSA studies (e.g. Benedetti et al. [2008], Sin et al. [2011]). Morris screening is an unbiased and computationally efficient method that indicates the significant parameters – an approach that we applied to double check the results from the SRCs method.

The primary objective of this study is to provide parameter sensitivity rankings for some of the key target output variables in SST/WWTP model calibration exercises (see Fig. 1) using the BSM2 platform. Furthermore, the study aims at assessing the impact of the 1-D SST model selection and two activated sludge hydraulic patterns on parameter sensitivity rankings for BSM2 outputs.

2 MATERIALS AND METHODS

2.1 WWTP modelling

All reported modelling and simulation was performed in Matlab (The Mathworks, Natick, MA). In the BSM2 implementation, we used both the model of Takács et al. [1991], further referred to as the 1-D^{1st} model, and that by Plósz et al. [2007], further referred to as the 1-D^{2nd} model. A modified version of the double-exponential settling velocity (v_s) expression of Takács et al. [1991] is used in both 1-D SST models that includes (i) the hindered settling parameter (r_H); (ii) the maximum settling velocity (v_0); (iii) the non-settleable fraction of the influent suspended solids (f_{ns}); and (iv) the settling parameter associated with the low concentration and slowly settling components of the suspension (r_P). Here, we also refer to r_H and v_0 as the Vesilind parameters. Further details on the model settings are shown by Ramin and Plósz [2012].

The WWTP layout and parameter values used in this study were presented by Jeppsson et al. [2007] and Sin et al. [2011], respectively. Biological wastewater treatment was modelled using the ASM No. 1 [Henze et al., 1987]. The selected Plant Performance Criteria (PPC) include the Effluent Quality Index (EQI) [Nopens et al., 2010], $X_{TSS,eff}$, reject water quality, methane production, total sludge production and the Operational Cost Index (OCI) [Nopens et al., 2010].

2.2 Description of the scenarios

Four scenarios have been used in this study, in terms of 1-D SST model structure and plant operation strategy, including:

- Scenario 1: 1-D^{2nd} SST model + WAS from the RAS stream;
- Scenario 2: 1-D^{2nd} SST model + WAS from the last aerobic reactor;
- Scenario 3: 1-D^{1st} SST model + WAS from the RAS stream;
- Scenario 4: 1-D^{1st} SST model + WAS from the last aerobic reactor.

The abbreviations, WAS and RAS, denote waste activated sludge and return activated sludge, respectively. The method using WAS from the last aerobic reactor is also referred to as the Garrett or the hydraulic method.

2.3 Uncertainty analysis

Monte Carlo simulation was chosen to analyze the influence of parameter uncertainty on the defined Plant Performance Criteria (PPC). The parameter space was defined by means of literature review and expert judgement. Because no *a priori* information was available, all model parameters were assumed to have a uniform probability distribution. When determining the range of the Vesilind settling velocity parameters, we used parameter values extrapolated to ranges that represent a moderate filamentous bulking scenario, i.e. diluted sludge volume index $DSVI_{max}$=200 mL g^{-1}. Since the Vesilind parameters are inherently correlated and cannot be sampled independently for individual Monte Carlo simulations, realistic couples of parameter values are calculated using a correlation formula [Plósz et al., 2011].

The upper and lower bounds of the biokinetic parameter distributions were assigned based on the uncertainty classifications given in Sin et al. [2009b]. The defined parameter space was sampled using Latin hypercube sampling (LHS) [Iman et al., 1981]. Parameter correlation was not considered during sampling as there is no prior information available. 500 samples were found sufficient to obtain a statistically acceptable Monte Carlo integration error on the mean of the PPC. Then, the Monte Carlo simulations with BSM2 were performed and the defined PPC were calculated based on time series data for each simulation. Finally, the average of the last 364 dynamic days of each calculated PPC was used for uncertainty and sensitivity analysis [Jeppsson et al., 2007].

2.4 Sensitivity analysis

Two methods were used for sensitivity analysis to independently cross-check the validity of sensitivity measures:

Linear regression of Monte Carlo outputs (SRCs Method): The standardized regression coefficients (SRCs) are obtained by performing a linear regression on each of the model outputs obtained from the Monte Carlo simulation:

$$sy_k = b_{0k} + \sum_{i=1}^{I} b_{k,i} \cdot \theta_i + \varepsilon_k \quad \text{for} \quad k = 1,2,..,K \tag{1}$$

sy_k is a vector of scalar values for the k^{th} model output, b_k is a vector of coefficients, θ is a matrix of parameter values (the sampling matrix) and ε_k is the error vector of the regression model. The dimensionless form of Eq. 1 using the corresponding means (μ_{syk},μ_θ) and standard deviations (σ_{syk},σ_θ) of the outputs and the parameters, respectively, results in SRCs of parameters that correspond to the k^{th} model output, y_k (β_k) [Sin et al., 2011]. The degree of linearization (R^2) obtained with the multivariate regression method indicates the reliability of the SRC values when used as an assessment of parameter sensitivity and it should be ≥0.7.

Morris screening: The Morris method relies on repeated computation of a local sensitivity measure called Elementary Effect (EE) at randomly selected points in the parameter space following an efficient sampling algorithm of Morris [Morris, 1991]. The EEs for each parameter are obtained from the following differentiation of the k^th^ model output (sy_k) with respect to the i^th^ parameter (θ_i):

$$EE_{i,k} = \frac{\partial sy_k}{\partial \theta_i} = \frac{sy_k(\theta_1, \theta_2, \theta_i + \Delta, \ldots \theta_M) - sy_k(\theta)}{\Delta} \tag{2}$$

where Δ is the predetermined perturbation factor of θ_i, $y(\theta)$ is the scalar model output evaluated at a point in the parameter space, while $y(\theta_1, \theta_2, \theta_i+\Delta, \ldots \theta_m)$ represents the scalar model output corresponding to a Δ change in θ_i. Each input is assumed to vary across p levels. The distribution of the EE for each input is obtained by performing the above calculation r times at randomly sampled points in the parameter space. In this study, Δ, p, and r are defined as 2/3, 4 and 15, respectively. Morris results are evaluated by comparing the mean and the standard deviation of the EE distributions for each parameter. The resilience of the Morris method with respect to type I errors (false positive), besides its low computational cost, makes this method an effective tool to identify significant parameters for further analysis [Sin et al., 2009a].

3 RESULTS

The SRCs obtained from the linear regression of Monte Carlo simulations are used as the sensitivity measures (β_i) of the parameters for each selected PPC. Scenario 1 with the 1-D^{2nd} SST model and RAS sludge wastage strategy serves as the base scenario. The parameters are ranked based on their sensitivity indices and the values are compared with the values from other scenarios. We only show parameters that at least in one of the scenarios have a $\beta_i \geq 0.1$ [Sin et al., 2011].
The importance rankings of uncertain parameters based on the variation of the economically related PPC are illustrated in Fig. 2. In all of the four scenarios, the prediction of the energy production capacity of WWTPs by means of the methane generated via sludge digestion is highly sensitive to heterotrophic yield (Y_H) and the Vesilind parameters. The predicted sludge production and the OCI are highly sensitive to r_H and v_0, as well as the inorganic content of TSS (X_{I2TSS}). Using the 1-D^{1st}, all the three target variables, shown in Fig. 2, are equally sensitive to Vesilind parameters and r_P (a calibration constant defining sludge settleability). The Y_H determines the ratio between the cells formed (and potentially anaerobically digested) per unit of degraded substrate (COD), and its highest importance on

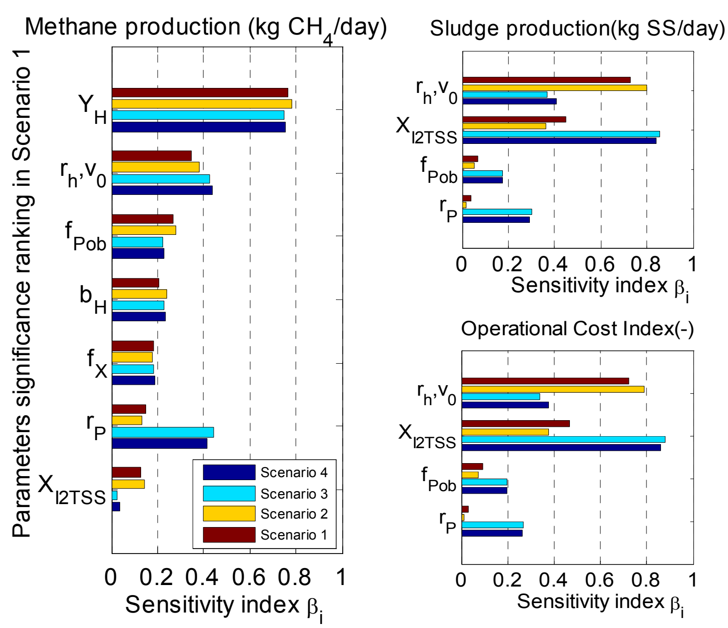

Figure 2. Parameter rankings for operational cost related plant performance criteria (PPC), based on SRC values.

predicting methane production agrees well with the process knowledge. Changes in r_H and v_0 strongly influence the overall sludge inventory in the activated sludge system. Thus, sludge production, methane generation and finally the total operational cost of the plant will also be affected. Finally, the X_{I2TSS} determines the TSS volume and thus the quantity of sludge to be disposed of. According to data shown in Fig. 2, the sludge withdrawal strategy influences, though not significantly, the significance ranking.

Parameter sensitivity ranking for predicting the Effluent Quality Index (EQI), $X_{TSS,eff}$ and NH_4 in reject water is shown in Fig. 3. In all scenarios, the EQI and $X_{TSS,eff}$ are the most sensitive to r_H and v_0 . This can be explained by their impact on the solids-liquid separation process behaviour and consequently on the plant's potential of particulate TSS pollution removal. Using the 1-D^{1st} model, the EQI and $X_{TSS,eff}$ target variables are equally sensitive to Vesilind parameters and r_P. In a lower order of magnitude, EQI shows sensitivity to nitrification (X_{I2TSS}, K_{OA} and K_{NH}) and denitrification (K_{OH} and ny_g) parameters. Reject water quality is mostly influenced by the inert content of TSS (X_{I2TSS}) and the heterotrophic yield coefficient (Y_H). This can be attributed to the influence that these two parameters have on: i) sludge production and ii) digester performance (biogas production). The absence of settling parameters here can be easily explained by: i) the slow dynamics of the anaerobic digestion system and ii) the high hydraulic retention time of the tank. Again, the sludge withdrawal mechanism does not change the results of the GSA.

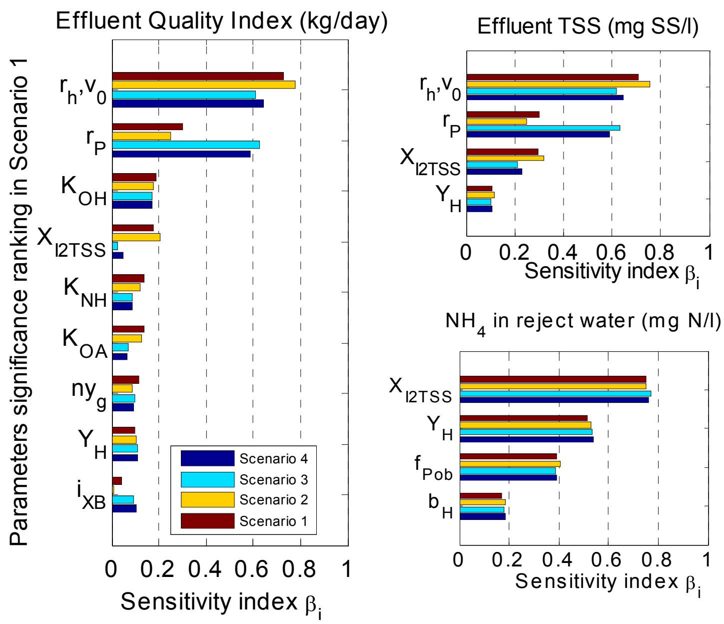

Figure 3. Parameter rankings for effluent quality related plant performance criteria (PPC), based on SRC values.

The validity of results obtained in the sensitivity analysis using the linear regression of Monte Carlo simulations is assessed using the Morris screening method. The obtained results are in close agreement showing the same top-ranked significant parameters. To demonstrate, Fig. 4 shows the estimated mean and standard deviation of the distribution of elementary effects of the model inputs for the key PPC: EQI and methane production in Scenario 1. In these plots, the wedge formed by the two lines corresponds to two times the standard error of the mean effects of the parameters on outputs given as $\mu_i = \pm 2x sem_i$ where $sem_i=\sigma_i/sqrt(r)$. These plots are helpful in screening the importance of parameters. Only if the parameter lies outside the wedge, then it is said to have a significant effect on the output. For methane production and EQI outputs, the significant parameters identified by Morris screening (the encircled parameters) are the same as the ones obtained on the basis of SRCs.

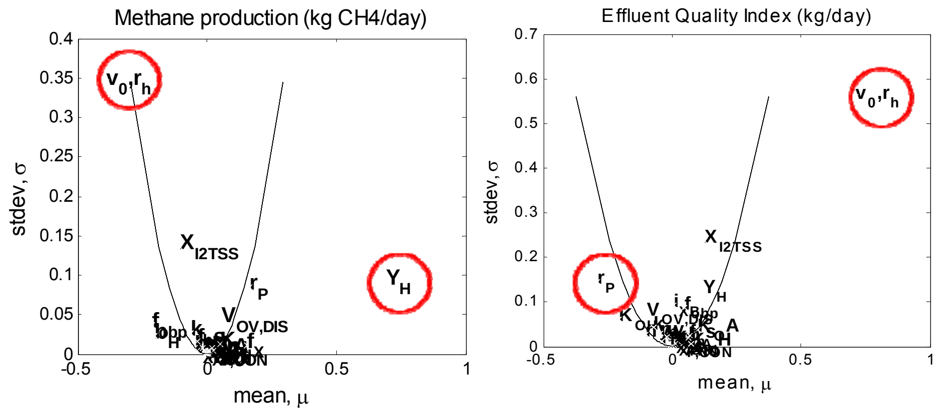

Figure 4. Morris screening results for scenario 1 on methane production and Effluent Quality Index (EQI).

4 DISCUSSION

The results of the GSA have implications on the optimal parameter selection for one-dimensional Secondary Settling Tank (1-D SST) model calibration exercises. To promote good SST modelling practice, based on most of the parameter sensitivity rankings obtained in this study, using 1-D^{1st}, calibration exercises should give equal importance to force calibrate (fine-tune) r_H, v_0 and r_P parameters. In contrast, for 1-D^{2nd}, the calibration exercises should primarily focus on providing realistic or directly measured r_H and v_0 parameters. In contrast to 1-D^{1st}, using 1-D^{2nd} in WWTP models, the relative sensitivity of most of the BSM2 model outputs to r_P is about one third of that obtained for r_H and v_0. In other words, the error introduced by practitioners not calibrating r_P in 1-D^{2nd} is significantly less than using 1-D^{1st} in WWTP models. We note that r_P cannot be measured, i.e. must be force calibrated using either type of 1-D SST model, and its value depends on the internal characteristics of SSTs. Furthermore, despite the fact that, compared to 1-D^{1st}, 1-D^{2nd} models contain more parameters (e.g., dispersion sub-model parameters), their relative sensitivity index is insignificant to the key target variables as shown in Figs. 2-4. However, under very high or very low flow conditions, the parameter sensitivity rankings will differ from results shown here. Importantly, these considerations only apply to model calibrations, whereby the real SST does not suffer from any significant internal malfunctioning.

5 CONCLUSION

The outcome of this sensitivity analysis study contributes to a better understanding of uncertainty in wastewater treatment plants, and explicitly demonstrates the significance of secondary settling processes in predicting the system performance.
First-order (1-D^{1st}) and second-order (1-D^{2nd}) secondary settling tank model parameters strongly influence biogas and sludge production, effluent quality and operational cost, but have an insignificant effect on nutrient-rich returns from the digester. The different hydraulic patterns do not change these results.
Using 1-D^{1st}, calibration exercises should give equal importance to estimate r_H, v_0 and r_P parameter values. Even though the 1-D^{2nd} secondary settling tank model has a higher number of parameters compared to the 1-D^{1st} model, calibration using 1-D^{2nd} models needs to focus mainly on providing realistic/measured values for the parameters r_H and v_0.

ACKNOWLEDGMENTS

The authors gratefully acknowledge funding for the study provided by the Danish Agency for Science Technology and Innovation, private companies, public utilities and universities engaged in the Storm- and Wastewater Informatics (SWI) project. Special thanks are due to Anitha K. Sharma, coordinator of SWI.

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