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Significance of uncertainties derived from settling tank model structure and parameters on predicting WWTP performance – A global sensitivity analysis study

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Abstract
Uncertainty derived from one of the process models – such as one-dimensional secondary settling tank (SST) models – can impact the output of the other process models, e.g., biokinetic (ASM1), as well as the integrated wastewater treatment plant (WWTP) models. The model structure and parameter uncertainty of settler models can therefore propagate, and add to the uncertainties in prediction of any plant performance criteria. Here we present an assessment of the relative significance of secondary settling model performance in WWTP simulations. We perform a global sensitivity analysis (GSA) based on Monte Carlo analysis in combination with multi-linear regression using four different simulation scenarios. We use the Benchmark Simulation Model Nr. 1 (BSM1), in which, we consider two operation scenarios for wastage of activated sludge (WAS), i.e. from the recycle of activated sludge (RAS) stream and from the last aerobic bioreactor upstream to the SST (Garrett/hydraulic method). For model structure uncertainty, two one-dimensional secondary settling tank (1-D SST) models are assessed, including a first-order model (the widely used Takács-model), in which the feasibility of using measured parameters for calibration is limited. The other SST model is a state-of-the-art, second-order, convection-dispersion tool (Plósz et al., 2007). The sensitivity results obtained from the four scenarios consistently indicate that the settler models and their parameters are among the most significant sources of uncertainty contributing to the predicted plant effluent data as well as sludge production and aeration demand, followed by influent wastewater fractions and biokinetic parameters, especially for autotrophs. Additionally, our results show that the first-order model systematically under-represents uncertainty. The outcome of this study contributes to a better understanding of uncertainty in WWTPs, and explicitly demonstrates the significance of secondary settling processes that are crucial elements of model prediction under dry and wet-weather loading conditions.

Keywords
Activated sludge wastewater treatment; global sensitivity analysis; one-dimensional modelling; secondary settling tank; Benchmark Simulation Model Nr. 1

INTRODUCTION

For model-based design, operation and optimisation of wastewater treatment plants (WWTPs), it is important to explicitly account for and to prioritize sources of uncertainty as well as to quantify their impact on performance criteria of WWTPs. Global sensitivity analysis (GSA) has been demonstrated as a valuable tool (e.g., Cierkens et al., 2010; Flores-Alsina et al., 2010; Sin et al.,

2011) to identify the most influential uncertainty sources. For activated sludge systems, the accurate assessment of solids inventory in bioreactors equipped with solid-liquid separator(s) is the most fundamental requirement of any model calibration procedure. Besides the influent concentration boundary conditions and biokinetic model parameters, the prediction of solids retention time and biomass composition are additionally influenced by the biomass settling behaviour and the SST model structure. Plósz et al. (2011) demonstrate that the solid-liquid separation related impacts can potentially propagate to the biokinetic model. For one-dimensional secondary settling tank (SST) models, Plósz et al. (2011) show that convection-dispersion models (e.g., Plósz et al., 2007, De Clercq et al., 2008), hereafter referred to as second-order models are superior to the first-order Takács-model (Takács et al., 1991) in describing the SST performance. Additionally, it is shown that the second-order model can effectively decrease the level of uncertainty introduced by the improper SST model structure. In contrast to the explicit (flow-dependent) dispersion used in convection-dispersion models, in the Takács model, it is not possible to control the dispersion term (see more on this in Plósz et al., 2011). Modellers using the Takács-model should thus compensate for the resulting error at the expense of forced (re-)calibration using unrealistic settling model parameters (Krebs, 1995). This is particularly true for simulation models run under wide ranges of flow boundary conditions, e.g., the Benchmark Simulation Model Nr. 1, BSM1 (Copp et al., 2002), and Nr. 2, BSM2 (Jeppsson et al., 2007). This also means that, using the popular Takács model, the feasibility of using measured parameters in the settling velocity function is limited.

As to predicting the sludge production and the effluent ammonium concentration in WWTPs, using a first-order 1-D SST model in the Benchmark Simulation Model Nr. 1, BSM1 (Copp et al., 2002), the ranking of uncertainty factors, compiled as a function of the sensitivity measures, show the highest significance for the TSS:COD ratio of sludge (F_TSS_COD) and the influent inert particulate COD fraction (Sin et al., 2011). Using a dissolved oxygen set-point control, it has additionally been shown that the most significant parameters for aeration energy demand are related to the prediction of sludge production. The question, thus, arises to what extent parameters of biokinetic and SST models are significant to model output, setting the main objective of this work.

Here, we present results obtained in a global sensitivity analysis using (i) first- and second-order SST models and (ii) two plant operation strategies for sludge wastage in the BSM1. These structural boundaries are used to set four simulation scenarios. The principal objectives of this work are (i) to assess the influence of model structure and operation strategy on the predicted uncertainty of selected plant performance criteria (PPC); (ii) to compare the influence of biokinetic and settling velocity parameters on selected PPC; and (iii) to assess the influence of parameters in the hydraulic sub-model of the convection-dispersion model on selected PPC. This work is accommodated in the Storm- and Wastewater Informatics project, SWI (www.swi.env.dtu.dk). In SWI, one of the goals is set to developing advanced model-based expert systems for on-line control of integrated urban wastewater systems (IUWS), in particular, under wet-weather conditions.

MATERIALS AND METHODS

WWTP modelling. The modelling and simulation platform WEST® (DHI, Denmark; Vanhooren et al., 2003) was utilised to carry out model simulations. In the Benchmark Simulation Model Nr. 1, BSM1 (Copp et al., 2002) implementation, we used the model by Takács et al. (1991), further referred to as the first-order model, and that by Plósz et al. (2007), further referred to as the convection-dispersion model. In the two SST models, the double-exponential expression for the settling velocity (v_S) by Takács et al. (1991) is used. The equation for settling velocity includes the hindered settling parameter (r_H) and the maximum settling velocity (v_0) – these former two are also referred to as the Vesilind parameters – the non-settleable fraction of the influent suspended solids, (f_{NS}) and the settling parameter associated with the low concentration and slowly settling components of the suspension (r_P). For the Takács-model, the 10-layer discretisation scheme is used. For the Plósz-model, a modified version of the double-exponential settling velocity function of Takács et al. (1991) is implemented, in which the maximum practical settling velocity parameter is omitted (Plósz et al., 2007). The Plósz-model includes a feedflow-dependent reduction factor in the downward convection term ($v_{F,C}$, critical SST feed velocity parameter) and the dispersion coefficient is governed as a function of the clarifier overflow velocity ($v_{Ov,C}$, critical SST overflow velocity parameter). Further details of the model are shown in Plósz et al. (2007, 2011).

WWTP model attributes, parameters and input. Uncertainty derived from the SST models was assessed as part of the pre-anoxic-aerobic activated sludge system (A_{SST}=1500 m^2; H_{SST}=4m; Q_{Under}=18831 $m^3 \cdot d^{-1}$; $Q_{Wastage}$=385 $m^3 \cdot d^{-1}$; Q_{Nitrat}=55338 $m^3 \cdot d^{-1}$) presented in the BSM1. The configuration of the modelled secondary treatment step includes a two-stage pre-anoxic and a three-stage aerobic zone, a secondary clarifier, nitrate- (Q_{Nitrat}) and sludge-recirculation streams (Q_{Under}), and excess sludge removal ($Q_{Wastage}$) from the sludge recirculation line. In the three-stage aerobic unit, dissolved oxygen concentration was controlled by using values of the oxygen mass-transfer coefficient (K_La) of 240 d^{-1}, 240 d^{-1} and 84 d^{-1}. Biological treatment was modelled using the Activated Sludge Model Nr. 1 (Henze et al., 1987). The input time-series data used for the WWTP simulation is based on the BSM1 simulation strategy, i.e. total length of time=150 days with constant dry weather to obtain a steady state condition. Additionally, this period is followed by twice the 14-day period, entailing dry- and wet-weather influent concentrations and flow data. The last 7 days of the dynamic simulations are used for the calculation of plant performance criteria. The PPC include the effluent concentrations of ammonium, nitrate, and total nitrogen, autotrophic (X_AUT) and total suspended solids concentrations, the effluent suspended solids concentration, as well as the sludge retention time (SRT), sludge production rate and the aeration energy consumption.

Description of the scenarios. Four scenarios have been used in this study, in terms of SST model structure and plant operation strategy, including

- Scenario1: Plósz-model+WAS from the RAS stream;
- Scenario 2: Plósz-model+WAS from the last aerobic reactor (Garrett/hydraulic method);
- Scenario 3: Takács-model+WAS from the RAS stream;
- Scenario 4: Takács-model+WAS via the Garrett/hydraulic method.

The abbreviation WAS and RAS denote wastage of activated sludge and recycle of activated sludge, respectively. Noteworthy is the fact that, in the BSM1, sludge wastage is carried out from the RAS stream, whereas, in the works by Sin et al. (2009, 2011), the Garrett/hydraulic method is implemented. For setting the range of the Vesilind settling velocity parameters, we used measured parameter value intervals presented by Plósz et al. (2011), including winter and summer data.

Uncertainty analysis. Forward Monte Carlo simulation was chosen to analyze the influence of parameter uncertainty on the defined PPC. Firstly, the parameters space was defined by means of literature review. Because of no *a priori* information was available, all the model parameters were assumed to have a uniform probability distribution. The upper and lower bounds of the biokinetic parameter distributions were assigned based on the three uncertainty classifications of the parameters by Sin et al. (2009), which corresponds to 5, 25 and 50% variation around the default values defined in the BSM1. The upper and lower bounds of the Vesilind parameters of settling velocity model were determined based on parameter values measured under winter and summer temperature conditions (Plósz et al., 2007, 2011). For each Monte Carlo simulation, couples of Vesilind parameter values were computed using correlation equations shown by Plósz et al. (2007). Secondly, the defined parameter space was sampled using Latin hypercube sampling (LHS). Parameter correlation was not considered during sampling. 500 samples are found sufficient to obtain reproducible PPC for the number of uncertain parameters in the BSM1 model. Thirdly, the Monte Carlo simulations of the benchmark simulation model (BSM1) were performed and the defined PPC were calculated based on time series data for each simulation. Finally, the mean and the variance of each PPC were calculated and used in the subsequent sensitivity analysis.

Sensitivity analysis. The standardized regression coefficients are obtained by performing a linear regression on each of the model outputs obtained from the Monte Carlo simulation:

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

$\mathbf{sy}_k$ is a vector of scalar values for the k^{th} model output, $\mathbf{b}_k$ is a vector of coefficients, $\boldsymbol{\theta}$ is a matrix of parameter values (the sampling matrix) and $\boldsymbol{\varepsilon}_k$ is the error vector of the regression model. Equation 1 can also be written in a dimensionless form using the corresponding means (μ_{sy_k}, μ_θ) and standard deviations ($\sigma_{sy_k}, \sigma_\theta$) of the outputs and the parameters, respectively (Saltelli et al., 2006):

$$\frac{\mathbf{sy}_k - \boldsymbol{\mu}_{sy_k}}{\boldsymbol{\sigma}_{sy_k}} = \boldsymbol{\beta}_k \frac{\boldsymbol{\theta} - \boldsymbol{\mu}_\theta}{\boldsymbol{\sigma}_\theta} + \boldsymbol{\varepsilon}_k \tag{2}$$

$\boldsymbol{\beta}_k$ is a vector of standardized regression coefficients (SRC) of parameters that correspond to the k^{th} model output, y_k. The degree of linearization (R^2) obtained with the multivariate regression method indicate the reliability of the SRC values to be used as an assessment of parameter sensitivity.

RESULTS AND DISCUSSIONS

In order to improve the understanding of results, presented in this study; we first recap some of the findings by Plósz et al. (2011), and then proceed to uncertainty and sensitivity analysis results. For the secondary clarifier, the 1-D model realism can be considerably compromised using the first-order Takács-model under the flow boundary conditions set in the BSM1 input time-series (14 days). The underlying reasons for this model behaviour are briefly summarised in the following. In terms of sludge blanket height (SBH), under moderate and high sludge loading conditions, its value can oscillate between relatively low and very high levels irrespective of the loading conditions applied, thereby introducing high uncertainty in solids inventory prediction. Values of sludge concentration in the sludge recirculation stream are considerably overestimated, under high and critical loading conditions. Using the Takács-model, the prediction of the effluent solids concentration using the measured Vesilind settling velocity parameters is deteriorated under all loading conditions. Under high and critical loading conditions, the under-prediction of the $X_{TSS,Eff}$ and the over-prediction of the solids' thickening behaviour, results in a significantly increased mass-flux recycled into the bioreactors.

Uncertainty analysis

Uncertainty analysis using different settler models in the BSM1. In Fig. 1, for the two different sludge wastage strategies, values of the variance (characterising uncertainty), obtained using the Takács-model in the BSM1, normalised to data obtained with the convection-dispersion SST model, are plotted for the selected nine PPC. We note that close to unity (shown with the red line), there is no difference between predicted uncertainties using either of the settler models. For the case of sludge wastage from the RAS stream, significant under-prediction of uncertainty using the Takács-model is obtained for sludge production, concentrations of TSS and the autotrophic biomass (X_AUT) in the bioreactor. This observation holds true, to a higher extent using sludge wastage from the last aerobic reactor (referred to as Garrett- or hydraulic-method). This can be explained by the overestimation of sludge retention in the system using the Takács-model under high and critical loading. For the effluent TSS concentration, uncertainty is significantly under-estimated using sludge wastage from bioreactor.

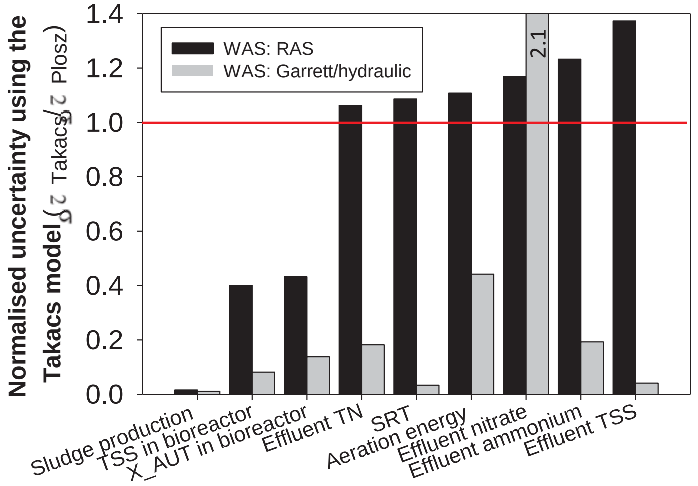

Figure 1 | Values of the variance for each PCC obtained using the first-order Takács-model in the BSM1, normalised to data obtained with the convection-dispersion SST model. The two different simulation model structures include sludge wastage via the last aerobic tank (Garrett-method) or via the RAS.

With wastage from RAS, uncertainties obtained in the effluent ammonium, nitrate and total nitrogen (TN) concentration predictions are comparable to that obtained using the Plósz-model – as expected since predicted variance of SRT are comparable in both settler models. This is not the case for the effluent total nitrogen concentration using the hydraulic wastage method, for which the variance is only about 20% of the predicted value using the Plósz-model.

Sensitivity analysis

Relative sensitivity of settling, biokinetic and influent parameters. In Fig. 2, for some selected plant performance criteria, we show the ranking of parameter significance in Scenario 1 as a function of absolute sensitivity measure (β_i) obtained for the first ten model parameters. Results obtained in Scenario 1 are compared with data deduced in Scenarios 2-4. For Scenario 1 and 2, using the convection-dispersion SST model, it is noteworthy that, compared to biokinetic and influent characteristics parameters, the significance of settling velocity parameters is the highest for all the performance criteria (except for SRT it is *F_TSS_COD*). Based on results obtained in Scenario 1 and 2, among the four settling velocity parameters, r_H and V_0 (Vesilind) parameters are found the most significant sources of uncertainties. Results obtained in Scenarios 1-2 show that the plant operation strategy (i.e. WAS strategies) can significantly influence the importance of parameters for all PPC. Taken together, these results overwhelmingly demonstrate the importance of settling velocity parameters. Additionally, they suggest the need of daily measurements, or some form of daily approximation of settling parameters; especially, should the plant models be used for supporting plant operation, optimisation and control purposes. A prerequisite of this approach, however, is to replace first-order SST models with state-of-the-art convection–dispersion models, in which measured settling velocity parameters can be readily used for model calibration.
In former studies, the Takács-model has only been used, and default settling velocity parameters has been chosen such that settling posed no real problems. Compared to results obtained in Scenarios 1-2, using the Takács-model, the top ranked parameters are altered only in the prediction of SRT, X_AUT, and the total biomass concentration in the last aerated bioreactor (TSS_biomass). In Scenarios 3-4), the relative significance of settling velocity parameters is consistently lower than those obtained in Scenarios 1-2. In Scenario 3-4, the order of parameter ranking is changed for all performance criteria. The predicted significance of the settling parameter r_P is significantly increased compared to that obtained with the Plósz-model.

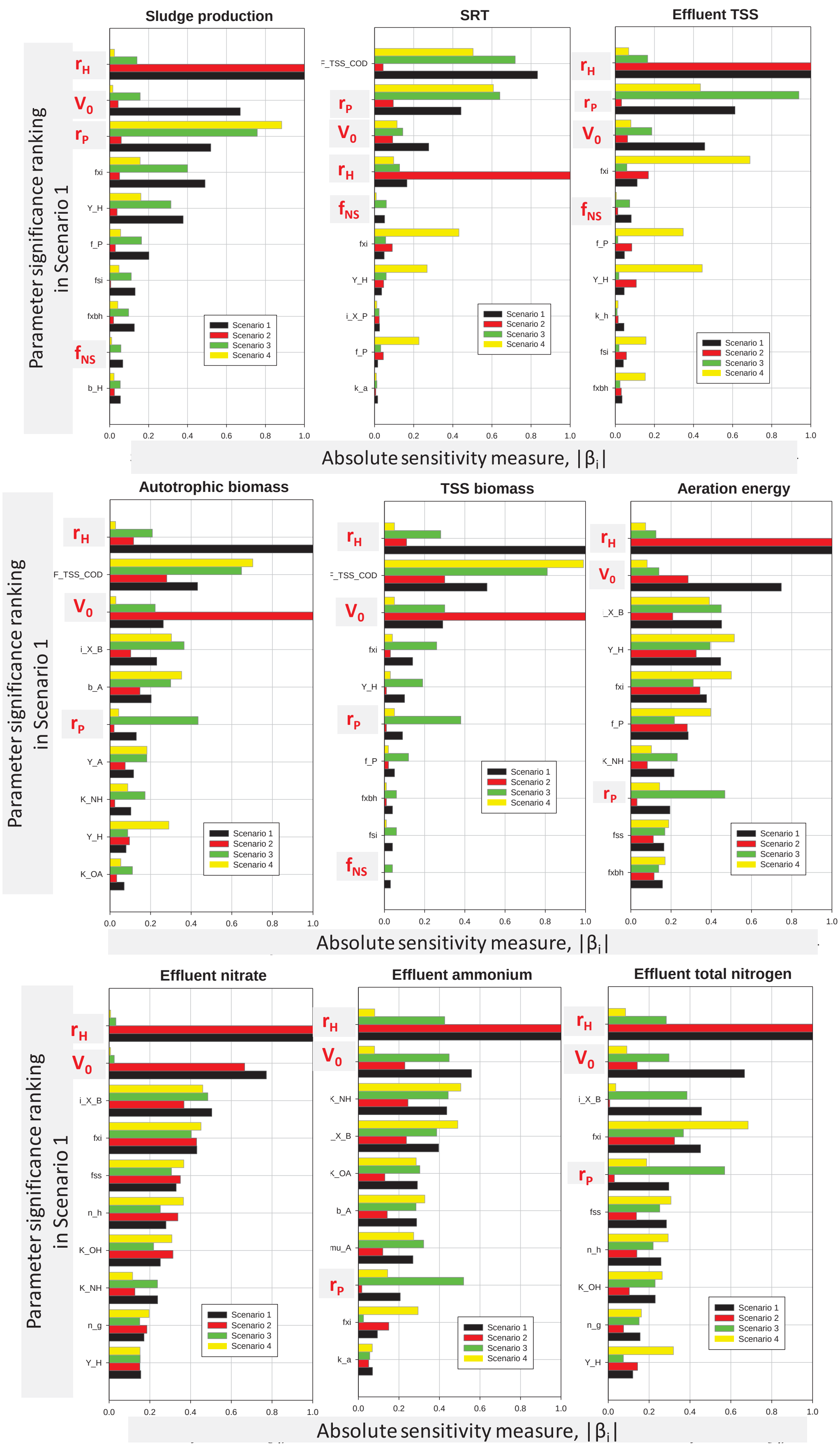

Figure 2 | Values of the relative sensitivity measure (β_i) plotted as a function of the first ten model parameters ranked in Scenario 1 for the nine plant performance criteria (PPC). Additionally, simulation

results obtained with the Plósz-model (Scenarios 2) and with the Takács-model (Scenario 3-4) are shown.
Relative sensitivity of SST hydrodynamic sub-model parameters. In Fig. 5, relative sensitivity measures obtained for two parameters - $v_{Ov,C}$ and $v_{F,C}$ – of the hydraulic sub-model of the Plósz SST model (i.e. Scenarios 1-2) are shown. We note that only those performance criteria are shown in Fig. 5, for which, β values are obtained above 0.1.

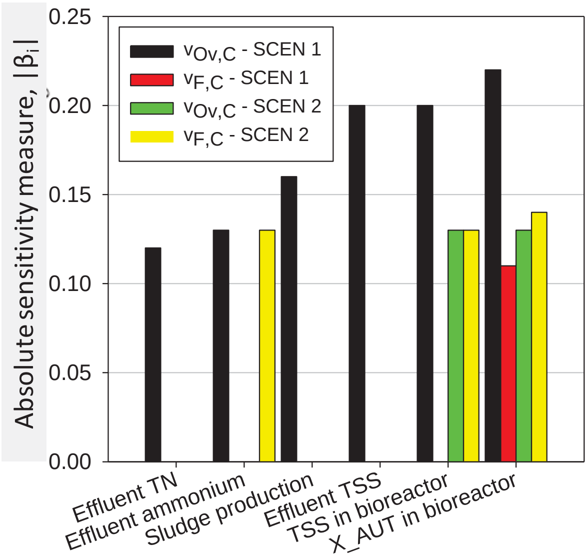

Figure 5 | Values of the absolute sensitivity measure (β_i), obtained for two parameters of the hydraulic sub-model of the Plósz-model (Scenarios 1-2), plotted as a function of the performance criteria, in which, β_i>1.

Although not as critical as settling velocity parameters, the sensitivity of six out of the PPC are significantly influenced by $v_{Ov,C}$ and $v_{F,C}$. It is noteworthy that the critical SST overflow velocity parameter is obtained as the most important hydraulic sub-model parameter. In the case of sludge wastage from the aerobic tank, the sensitivity of TSS and X_AUT concentrations in bioreactor to $v_{Ov,C}$ are still significant. Taken together, calibration of the hydraulic SST sub-model is an important part of activated sludge modelling – a task that can be executed using numerical experimental results obtained with computational fluid dynamics models (De Clercq, 2003; Plósz et al., 2007).

CONCLUSIONS

To quantify the uncertainty related to model parameters, one would expect that the uncertainty derived from the model structure itself should be significantly lower than that related to model parameters. Settler models and settling model parameters were not subject to uncertainty analysis in any former studies and in BSM1. This work extends the focus to the secondary settler. The concluding remarks of this work are summarised as follows:

- Settler models and their parameters are found the most significant sources of uncertainties, impacting the plant performance criteria, followed by influent wastewater fractions and biokinetic parameters related to autotrophs.
- As regards to model structure uncertainty, the Takács-model consistently tends to overestimate the solids inventory in the system, compared to the Plósz-model. This discrepancy becomes more pronounced in the case of sludge wastage from aeration tanks. In this case, the Plósz settler model indicates *correctly* significant impact on the biological plant performance (as well as solids production and aeration energy) due to settler model performance uncertainties.
- Based on the sensitivity analysis results, we conclude that the daily measurement, or some form of daily approximation of settling parameters is needed to be carried out in the future; should the plant models be used for supporting plant operation, optimisation and control purposes. A

prerequisite of this approach is to replace first-order SST models with state-of-the-art convection–dispersion models. This is an especially significant message to the benchmarking community that can contribute to a better understanding of the results obtained thereof.

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