Shall we upgrade one-dimensional secondary settler models using in WWTP simulators? Yes.

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Abstract

In this paper, we present an assessment of two one-dimensional (1-D) secondary settling tank (SST) models that are based on hyperbolic (Takács et al., 1991) and parabolic (Plósz et al., 2007) partial differential equations. The former model is currently the most widely used by process modellers, whereas the latter model is a mathematically sound, convection-dispersion model. Simulation results obtained for the suspended solids concentration in the effluent ($X_{TSS,Eff}$) and in the sludge recirculation stream (X_{TSS,RAS}) and the sludge blanket height (SBH) values are first used to demonstrate the behaviour of the two 1-D SST models. A scenario analysis is carried out using different values of SST feed flow rate (Q_{Feed}), 20-51 m·d⁻¹, underflow (sludge recirculation) rate (Q_{Under}), 10-25 m·d⁻¹, i.e. surface overflow rate (Q_{Over}), 10-26 m·d⁻¹, and feed solid concentration ($X_{TSS,Feed}$), between 2-4.5 g·L⁻¹. Solids loading rates used in the simulations range from 1.81 to 0.56 km m⁻² h⁻¹. 9.56 kg·m⁻²·h⁻¹. We additionally present a correlation assessment for settling parameters, and the obtained the equations were used to estimate settling velocity parameters in the simulation studies. In an integrated wastewater treatment plant (WWTP) model, the impact of 1-D SST model selection on the overall simulation performance is evaluated using the benchmark simulation model Nr. 1 (BSM1) by Copp et al. (2002). We assess the impact of liquid temperature on model prediction, in terms of solids inventory in the bioreactors, nitrogen removal and solids retention time as a function of the solids settling behaviour. Compared to measured and numerical (CFD) experimental as well as to literature data, results obtained in the scenario analysis and WWTP modelling suggest that the hyperbolic model, describing the SST, can introduce significant errors into WWTP model prediction. These impacts can be effectively mitigated using convectiondispersion models that the authors of this paper thus advocate to employ in WWTP simulators.

Keywords

Activated sludge; secondary settling tank; one-dimensional modelling; solids settling parameters; scenario analysis; WWTP modelling

INTRODUCTION

In WWTP simulation environments, biological process models are mostly combined with onedimensional 1-D SST models. A 1-D model of the setter is inherently a simplification of the real system and of the underlying processes (e.g., gravity- and compression settling, viscosity, dispersion, upward and downward convection, sludge collection mechanisms), taking place in a three-dimensional reactor. To obtain an effective simulation performance in 1-D, it is crucial that the SST model accounts for some of the important fluid dynamical processes. The 1-D SST model identification/calibration is not a trivial process, and it requires sound mathematical solutions and experimental observations. To simulate the hydrodynamics of secondary clarifiers, computational fluid dynamic (CFD) models can be applied, e.g., the one developed by Weiss et al. (2007). Implementation of CFD models coupled with activated sludge simulators, where 1-D clarifier models are mostly used, is computationally still too expensive. One way to overcome this problem is by calibrating 1-D models using numerical experimental data obtained using 2-D or 3-D hydrodynamic models – an approach first advocated by DeClercq (2003). In order to implement this method for the first time, Plósz et al. (2007) used CFD simulation results, obtained with the Weissmodel, to develop a 1-D SST model. Using this model, an optimised approximation of the solids profile in a flat-bottom SST can be achieved, thereby also improving the prediction of X_{TSS,Eff}

concentration and solids thickening under a broad range of flow conditions, including critical overloading (Plósz et al., 2007). Despite the progress made in the last two decades in the field (Watts et al., 1996; Diehl and Jeppsson, 1998; Bürger et al., 2005; Plósz et al., 2007; DeClercq et al., 2008), the 1-D SST model developed by Takács et al. (1991) is still the most widely used. This can, in part, be explained by the facts that most of the software packages provide only the Takácsmodel, and that process modellers do not necessarily have the background and the ability to assess other approaches. A drawback of this model, resting on a hyperbolic continuity equation, is the fact that the solids concentration depends only on the height of the layer (z), but not on the concentration gradient. Moreover, in the Takács-model, the rough discretisation (10 layers) of the first-order model introduces sufficient "numerical dispersion" to find a smooth concentration profile (Takács, 2008). That is the introduction of some numerical error makes the model behave as a second order convection-dispersion model - a mathematically unacceptable solution. A common feature of the more recent 1-D SST models developed is that they all incorporate a second-order derivative in the mass-transport equation, i.e. they are based on a parabolic partial differential equation (PDE). The second order derivative term can account for compression settling and/or solid dispersion. The latter process can be characterised with a dispersion coefficient (D_c) that is a characteristic to the surrounding medium and is always connected to flow processes. D_C is independent of molecular properties, and should thus not be confused with diffusion. In 1-D clarifier models, the dispersion term implicitly accounts for several effects, such as turbulent diffusivity, 2-D and 3-D dispersion, as well as anomalies in the particulate transport, the sludge removal procedure, and errors introduced by the numerical method Furthermore, the introduction of the dispersion term helps to distinguish between effects of sludge settleability and other effects (Ekama et al., 1997). The question arises how the model selection for representing the SST in an integrated wastewater treatment plant (WWTP) model can influence the overall simulation performance -a focus chosen for this paper. In order to assess the behaviour of SST by 1-D models, we rely on experimental and numerical observations presented in literature. Ekama et al. (1997) show that as the sludge blanket grew deeper, the X_{TSS Eff} levels rose. In a review article, Parker et al. (2001) confirm that higher sludge blanket heights (SBH) translate to higher effluent suspended solids based on modelling and field studies. Proper activated sludge system operation and good secondary clarifier design results in average $X_{TSS,Eff}$ concentrations of 10 g·m⁻³. Recommended design guidelines, e.g., that by the North-American Environmental Protection Agency encourages solids loading rate (SLR) values up to 10 kg·m⁻²·h⁻¹. The available information on maximum demonstrated SLR capacity of the types of tanks, commonly used in the United States (Ekama et al., 1997) show on values for Circular (flocculator, suction), Circular (flocculator, scraper), Rectangular (Gould Type 2) and Rectangular (Gould Type 1) of 8.3, 7.6, 6.5 and 4.6 kg·m⁻²·h⁻¹, respectively. These values are considerably lower than the recommended value, and establishing relative SLR capacity for each clarifier type thus is a high priority research (Parker et al., 2001). Moreover, in contrast to popular belief, in SSTs with flocculator centre or with sufficient mixing around the inlet area, resulting in effective flocculation process, the increasing sludge volume index (SVI) can increase the SBH, but cannot decrease the $X_{TSS,Eff}$ (Parker et al., 2001). Within the SVI range 25–150 ml·g⁻¹, no significant correlation can be observed between SVI and X_{TSS.Eff}. For the systems reported by Parker et al. (2001) with/without flocculator centre, X_{TSS,Eff} varies between 6-18 g·m³ under low and moderate solids loading conditions.

In order to optimise the description of real systems and deterministic model predictions in widely used WWTP simulators, we hereby initiate a discussion via a series of papers, out of which, this study represents the first step. The principal aim of the present work is to give an assessment of the widely used Takács-model and of a convection-dispersion settler model, used in WWTP models. Numerical experiments are carried out in scenario simulations using a range of SST feed and underflow rate values as well as feed solids concentrations.

Clarifier grid points \rightarrow	<i>i</i> =1	1 <i<f< th=""><th>i=f</th><th>f<i<sc< th=""><th>$sc \le i < n$</th><th>i=n</th><th></th></i<sc<></th></i<f<>	i=f	f <i<sc< th=""><th>$sc \le i < n$</th><th>i=n</th><th></th></i<sc<>	$sc \le i < n$	i=n	
Solids fluxes, $\left(\frac{\partial C}{\partial t}\delta z\right)\downarrow$	Effluent grid point	Grid points in the clarification zone	Feed grid point	Grid points in the thickening zone	Grid points with sludge withdrawal	Bottom grid point with sludge withdrawal	Rate equations
1. Gravity settling	$-v_{S,i}C_i$		$v_{s,i}$	$_{-1}C_{i-1} - v_{S,i}C_i$		$v_{S,i-1} \cdot C_{i-1}$	$v_{S,i} = v_0 \left(e^{-r_H (C_i - f_{NS} \cdot C_F)} - e^{-r_p (C_i - f_{NS} \cdot C_F)} \right)$
2. Convective movement in the clarification zone	$U_{Up}C_{i+1}$	$U_{Up}(C_{i+1}-C_i)$	$-U_{Up}C_i$				$U_{Up} = \frac{Q_{Over}}{A_{SST}}$
3. Convective movement in the thickening zone			$-U_{Dn}C_i$	U _{Dn}	$(C_{i-1}-C_i)$	$U_{Dn}C_{i-1}$	$U_{Dn} = \frac{Q_{Under}}{A_{SST}} \cdot \eta_{C}$, where $\eta_{C} = \begin{bmatrix} \eta_{C,0} & \text{if } v_{F} < v_{F,C} \\ \min\left\{\eta_{C,0} + \left(\frac{v_{F} - v_{F,C}}{v_{F,C}}\right)^{2}; 1\right\} & \text{if } v_{F} \ge v_{F,C} \end{bmatrix}$
		Ι	$D_{C,i}(C_{i+1}$	$-C_i$)			$D_{C,i} = \frac{D_C}{s_T}$
4. Solids dispersion				$D_{C,i}(C_{i-1}-c)$	C_i)		$D_{C} = \begin{cases} D_{C,0} & \text{if } v_{Ov} < v_{Ov,C} \\ D_{C,0} + \gamma (v_{Ov} - v_{Ov,C})^{2} & \text{if } v_{Ov} \ge v_{Ov,C} \end{cases}$
5. Clarifier inflows and outflows	$-v_{Ov}C_i$		$v_F C_F$		$-v_{Un,i}C$		$v_{Ov} = \frac{Q_{Over}}{A_{SST}} \qquad v_F = \frac{Q_{Feed}}{A_{SST}} \qquad v_{Un,i} = \frac{Q_{Under,i}}{A_{SST}},$ and $Q_{Under} = \sum_{i=sc}^n Q_{Under,i}$

Table 1. The difference scheme of the ODEs obtained in the discretisation of the PDE presented by Plósz et al. (2007), where X_{TSS} is denoted as C_i

Correlation equations, describing the sludge settling velocity function parameters as a function of the settling volume, are assessed using measured data. In addition, we assess the impacts of 1-D SST models on the simulation results obtained in an integrated dynamic WWTP model that, in most part, rests on the activated sludge benchmark simulation model No. 1 (BSM1).

MATERIALS AND METHODS

Batch settling experiments. Batch settling curves were measured using the SettloMeter (Applitek NV, Belgium; Vanrolleghem et al., 1996), and further information on the experimental techniques used is presented by Plósz et al. (2007).

Simulation studies. The modelling and simulation platform, WEST® (MOSTforWATER NV, Belgium; Vanhooren et al., 2003) was utilised to carry out transient-to-steady-state and dynamic model simulations using the model by Takács et al. (1991), hereby referred to as the first-order model and that by Plósz et al. (2007), referred to as a convection-dispersion model. The CFD model and the numerical experiments, used to obtain the steady-state CFD simulations shown in this paper, are presented elsewhere (Plósz et al., 2007; Weiss et al., 2007).

First-order model. A dynamic model of the clarification/thickening process is presented by Takács et al. (1991). The hyperbolic PDE, describing the mass transport in the settler, is discretised using 10 horizontal layers. The novelty of this model is that it proposes a double-exponential expression for the settling velocity (v_s) which is valid for both the thickening and the clarification zone. The equation for settling velocity includes the hindered settling parameter r_H , the maximum settling velocity (v_o), the non-settleable fraction of the influent suspended solids, C_F , (f_{NS}) and the settling parameter associated with the low concentration and slowly settling components of the suspension (r_P). In this study, we use the 10-layer representation, described in the original paper that is also implemented in the BSM1 (Copp et al., 2002).

Convection-dispersion model. In Table 1, the result of discretising the parabolic PDE into a set of ordinary differential equations (ODEs) by differencing the spatial derivatives of the PDE is shown in a matrix format, originally proposed by Plósz et al. (2007). In the Gujer-matrix, also known as the Petersen matrix, often used to represent activated sludge models, the stoichiometric coefficients are shown in the matrix elements. Conversely, in the difference scheme, shown in Table 1, in the set of matrix elements, associated with each model layer or grid point (i), the local solids fluxes, i.e. the local concentration values multiplied by the different solids transport process rates are shown. A modified version of the double-exponential settling velocity function of Takács et al. (1991) is implemented in this settler model, in which the maximum practical settling velocity parameter is omitted (Plósz et al., 2007). For every Δt , density currents are taken into account by positioning the feed layer i=f above the first layer that has a concentration greater than $X_{TSS,Feed}$. Furthermore, according to preliminary model evaluations, at high clarifier loads, if the feed layer is positioned above a certain depth, the 1-D model under predicts most of the solids profile obtained with the CFD model (data not shown).We found that this drawback can effectively be overcome in the 1-D model, by restricting the maximum height of the feed layer to 53% of the clarifier depth. A possible explanation of this behaviour is that the turbulent fluid motions, prevailing under SST overloading can effectively dilute the influent current in a relatively short horizontal distance from the influent point, and its impact on the average vertical solids concentration values, used for 1-D model evaluation, can thus become negligible. We have found a number of 60 grid points sufficient to compute concentration profiles that are independent of the discretisation scheme and to keep the computational efforts to a minimum. The feed-layer thus is limited to a depth at the layer 32. We note that, for the Takács-model, at finer discretisations, e.g., using 60 layers, the simulation performance is worse than with using only 10 layers (Watts et al., 1996). Furthermore, the 1-D SST model includes a feedflow-dependent reduction factor in the downward convection term (η_c) and the dispersion-coefficient is governed as a function of the clarifier overflow velocity (see Plósz et al., 2007). Minimum settling flux conditions are formulated above and below the feed layer using the Godunov scheme, see e.g., Diehl and Jeppson (1996). We note that DeClercq et al. (2008) used the Engquist and Osher flux. The fourth-order Runge-Kutta numerical integration method with variable time step size was used for the numerical integration of the stiff ODE system. Further details of the model description can be found in Plósz et al. (2007). We finally note that the extra computational demand of using second-order models, e.g., the convection-dispersion model used in this paper, instead of first-order ones, should not represent any significant obstacle for process modellers, in terms of additional computational time.

Scenario simulations. Scenarios were simulated in a case study using a secondary clarifier with a horizontal surface area, A_{SST} =1000 m² and vertical depth, H_{SST} =3 m. In the transient-to-steady-state simulations, we used three independent initial conditions, in terms of flow and solids concentration, in a four-level factored experimental plan, shown in Table 2.

-	Q _{Feed}	Q _{Under}	X _{TSS,Feed}
	$(m^3 \cdot d)$	$(m^3 \cdot d)$	$(kg \cdot m^3)$
1	20000	10000	2.2
2	35000	15000	3
3	45000	20000	4
4	51000	25000	15

Table 2 | Boundary conditions used in all possible combinations for the scenario analysis

For the simulations, the settling model parameters used are $v_0=100.5 \text{ m}\cdot\text{d}^{-1}$; $r_H=0.287 \text{ m}^3 \cdot \text{kg}^{-1}$; $r_P=10 \text{ m}^3 \cdot \text{kg}^{-1}$; $f_{NS}=0.00138$; $D_{C,0}=3.95 \text{ m}^2 \cdot \text{d}^{-1}$; $\gamma=2.2 \cdot 10^{-2}$; $v_{Ov,0}=15 \text{ m}\cdot\text{d}^{-1}$; $\eta_{C,0}=0.5$; $v_{F,C}=30.5 \text{ m}\cdot\text{d}^{-1}$.

WWTP modelling. We assessed the two 1-D SST models in a simulation environment, including a pre-anoxic-aerobic activated sludge system (A_{SST} =1500 m²; H_{SST} =4m; Q_{Under} =18831 m³·d⁻¹; $Q_{Wastage}$ =385 m³·d⁻¹; Q_{Nitrat} =55338 m³·d⁻¹) presented in the BSM1 (Copp, 2002). 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. In the BSM1, for the pre-anoxic zone, oxygen mass-transfer through the liquid surface (Plósz et al., 2003) is not accounted for, i.e. K_La =0. Biological treatment was modelled using the Activated Sludge Model Nr. 1 (Henze et al., 1987) with parameter values presented by Spanjers et al. (1998). The input time-series data used is presented by Copp (2002). Temperature dependency of kinetic parameters was modelled using Arrhenius-coefficient values by Melcer (2003). We note that our model does not account for the impact of temperature on sludge viscosity that may well be a significant factor, influencing the overall solids settling.

RESULTS AND DISCUSSIONS

Scenario simulations

In Fig. 1, scenario simulation results obtained for sludge blanket height (SBH), total suspended solids concentration in the recirculation stream ($X_{TSS,RAS}$) and in the clarifier overflow ($X_{TSS,Eff}$) are plotted as a function of SST mass-loading specific to the underflow rate, $\varphi=X_{TSS,Feed}\cdot Q_{Feed}/Q_{Under}$. At φ values between 2.2 and 10 kg·m⁻³, compared to results obtained with the Plósz-model, data derived from simulations using the Takács-model indicate (i) 0.8 to 7.0 times higher SBH values; (ii) up to 10% higher values of $X_{TSS,RAS}$; and (iii) up to 7 times higher $X_{TSS,Eff}$. For $10 \le \varphi \le 20$ kg·m⁻³, simulation results obtained with the Takács-model show 1 to 1.5 times higher $X_{TSS,RAS}$, 0.06 to 0.67 times lower $X_{TSS,Eff}$, 0.68 to 0.98 times lower SBH values than those obtained with the Plósz-model. Within the $2.2 \le \varphi \le 20$ kg·m⁻³ interval, SBH values correlate well with the $X_{TSS,Eff}$ using the Plósz-model that is in close agreement with literature data. Effluent total suspended solids concentration values ($X_{TSS,Eff}$) obtained using the Plósz-model show a break-through, i.e. sludge wash-out event,

characterised with an inflection-point at $\varphi=10 \text{ kg}\cdot\text{m}^{-3}$. For $X_{\text{TSS,Eff}}$ values, results obtained with the Takács-model indicate a diffuse transition from $\varphi=2$ to 15 kg·m⁻³ without showing any break-through. A striking thing about the SBH obtained with the latter model is that, for $2.2 \le \varphi \le 10 \text{ kg}\cdot\text{m}^{-3}$, its value can only take either 0.6 or 2.1 metres irrespective of the loading conditions applied in the scenario analysis. This factor can introduce significant uncertainties in calculating the sludge inventory in the SST. Values of $X_{\text{TSS,RAS}}$ obtained with the Takács-model, plotted at $\varphi>10 \text{ kg}\cdot\text{m}^{-3}$, suggest an overestimation of solids thickening, and thus very high concentration levels in the recycle stream. Using the convection-dispersion model, such simulation inefficiency can effectively be avoided.



Figure 1 | Values of the sludge blanket height (SBH), total suspended solids concentration in the recycle/under flow ($X_{TSS,RAS}$) and in the effluent/over flow ($X_{TSS,Eff}$). The scenario analysis was carried out using the two 1-D SST models for a hypothetical SST (A_{SST} =1000 m²; H_{SST} =3 m). Steady-state CFD simulation results were obtained for a flat-bottom SST (A_{SST} =855 m²; H_{SST} =3 m). Measured values were obtained in two conical SSTs (Heist: A_{SST} =254 m²; $H_{SST, side-wall}$ =1.92 m; $H_{SST, centre}$ =2.41 m; Essen: A_{SST} =292 m²; $H_{SST, side-wall}$ =1.88 m; $H_{SST, centre}$ =2.56 m).

Under critical loading conditions, i.e. at φ >10 kg·m⁻³, simulation results obtained for X_{TSS,Eff} using the Takács-model are significantly lower than those obtained with the Plósz-model. According to the literature, X_{TSS,Eff} values obtained with the Takács-model at φ <10 kg·m⁻³ suggest an overestimation of a properly designed and functioning SST effluent quality that is not the case for the Plósz-model. For 5.13< φ <13.4 kg·m⁻³, Plósz et al. (2007) investigate the performance of an SST (A_{SST}=855 m²; H_{SST}=3 m) using the 2-D CFD model by Weiss et al. (2007), evaluated and confirmed using measured data. In Fig. 1, steady-state results obtained with the CFD model under

moderate, high and critical SST loading conditions, are in good agreement with the simulation results obtained using the convection-dispersion model, in terms of SBH, X_{TSS,RAS} and X_{TSS,Eff}. For $3.45 < \phi < 24.3 \text{ kg} \cdot \text{m}^{-3}$, De Clercq (2006) presents steady-state data measured in two conical SSTs (characteristics shown in Fig. 1). We note that, for the 1-D scenario simulations, we only used one set of settling velocity parameters, whereas the measured data was obtained in a wide range of SVIs. At $\rho < 6.5 \text{ kg} \cdot \text{m}^{-3}$, the measured SBH values are significantly higher than the 1-D simulation results obtained using the convection-dispersion model. This result agrees well with data presented by Parker et al. (2001), who conclude that SBH values are typically higher in conical SSTs with scraper than in flat-bottom settlers equipped with organ-pipes. Measured SBH values obtained are at around 1.9-meter distance from the liquid surface that is approximately equal to the side-wall depths of these SSTs. Furthermore, these two SSTs have a 0.5-1 meter shallower centre-depth than the other SSTs considered, which can additionally explain the deviation. At $\varphi < 6.5 \text{ kg} \cdot \text{m}^{-3}$, for reasonably well settling sludge, i.e. SVI<150 ml·g⁻¹, measured X_{TSS,RAS} and X_{TSS,Eff} data show a close agreement with the simulation results obtained with the Plósz-model. We note that the X_{TSS Eff} value is influenced by factors, such as flocculation processes, that are not explicitly accounted for by any of the models studied and that can effectively deteriorate the model prediction. For $6.5 < \varphi < 13.5$ kg·m⁻³, the measured data are in excellent agreement with the simulation results obtained using the convection-dispersion model, in terms of SBH, X_{TSS,RAS} and X_{TSS,Eff}. Under severe SST over-loading, φ ~24 kg·m⁻³, the measured SBH is somewhat lower than the model approximation that can, in part, also explain the higher $X_{TSS Eff}$ value, simulated with the 1-D SST models. For SVI<150 ml·g⁻¹, despite the severe over-loading and the different geometrical characteristics of the SSTs considered, the simulated (Plósz-model) and measured X_{TSS RAS} results are in excellent agreement, as a result of the effective prediction of the sludge thickening behavior, under extreme operating conditions.

Relationships between solids settling parameters

The stirred specific volume index (SSVI_{3.5}) was assessed in a measurement campaign, taking place under relatively cold (12-15 °C) and warm (~20 °C) liquid temperatures. Values obtained are in the range 70-105 L·kg⁻¹ (Fig. 2). They are smaller than values for the diluted sludge volume index (DSVI) by a factor of 0.64±0.22. This value agrees well with the factor of 0.67 given by Ekama et al. (1997).



Figure 2 | Values of solids settling parameters plotted as a function of stirred specific volume index.

Values obtained for v_0 and r_H are shown to correlate reasonably well with the SSVI_{3.5} using the general equations by Ekama et al. (1997). Data obtained indicate some but no significant temperature dependence of v_0 and r_H .

$$v_0 = \alpha \exp(-\beta \times SSVI_{3.5}) \tag{1}$$

$$r_{H} = \kappa + \lambda \times SSVI_{3.5} \tag{2}$$

We have found values of 133.7 m d⁻¹ and 3.4 kg m⁻³ for α and β , respectively. The correlation for v_0 shows that this parameter is practically independent of the SSVI_{3.5}, and $v_0 \sim \alpha$. Values obtained for λ and κ are 0.0026 m³ l⁻¹ and 0.0628 m³ kg⁻¹, respectively. These results are in close agreement with the data reported by Ekama et al. (1997). To the authors' opinion, however, such correlations should be used with care for their theoretical background is unclear (see e.g., Dick and Vesilind, 1969) that can be demonstrated with the non-correlating data plotted in Fig. 2.

WWTP modelling

Clarifier performance. In the WWTP simulations using the BSM1, the solids settling velocity parameters were calculated for an array of DSVI values, 50-200 ml·g⁻¹ using the correlations Eq. 1 and Eq. 2. In our simulation model, compared to the default settings in BSM1, the r_P and f_{NS} parameter values are changed to 10 m³·kg⁻¹ and 0.00138, respectively, as shown by Plósz et al. (2007). A sequence of the default input-time series, including nine times the 14 days of influent data, is implemented using DSVI values set for each 14-day period. In Fig. 3, values of SBH, X_{TSS,RAS} and X_{TSS,Eff} obtained are plotted as a function of the time elapsed and of the DSVI.



Figure 3 | Values of the sludge blanket height, X_{TSS,RAS} and X_{TSS,Eff} obtained with the BSM1.

As a function of the progressively deteriorating sludge quality (days 0-42), the Takács-model shows a "fuzzy" prediction of the SBH – an impact that can severely deteriorate the assessment of sludge retention time (SRT) in the system (see Fig. 4). This is not the case for the Plósz-model that suggests a gradually increasing, i.e. more realistic, blanket depth. For DSVI=150 and 200 ml·g⁻¹ (days 43-70), sludge thickening deteriorates, thereby also decreasing $X_{TSS,RAS}$ values. Using the Plósz-model, simulation results suggest approximately 1000 and 1500 g/m³ lower values on average than the Takács-model. For 50 \leq SVI \leq 150, values of $X_{TSS,Eff}$ are between 15-80 g·m⁻³ that is significantly higher than that reported in literature (see introduction) and than that simulated by the Plósz-model. In this SVI range, $X_{TSS,RAS}$ values predicted by the two models do not deviate significantly. Between days 56 and 70, as a result of dispersion, severe sludge wash-out is predicted by the Plósz-model, $X_{TSS,Eff}$ values up to 800 g·m⁻³, which is not the case for the Takács-model that predicts $X_{TSS,Eff}$ values only up to 270 g·m⁻³.

Biological treatment. In Fig. 4, the calculated difference between the simulation output statevariables obtained using the Takács- and the Plósz-model are plotted. The selected state-variables are the total suspended solids concentration in the last aerobic reactor ($X_{TSS,In}$), autotrophic biomass concentration (X_{AUT}) and ammonia-ammonium, nitrate and total nitrogen concentrations. Additionally, we show the difference between the SRT calculated in the dynamic simulations using the two models. The SRT value, calculated for each Δt , is the instantaneous solids mass retained in the system (bioreactors and SST) over the solids wastage rate. The sludge age is conventionally used as a steady-state property, and Takács (2008) present a method to calculate the dynamic SRT of activated sludge systems. For the benchmark parameter setting (left column in Fig. 4), under critical operating conditions (days 42-84), compared to the simulation results obtained using the Plósz sub-model, values of the $X_{TSS,In}$ and X_{AUT} are both increased in the bioreactors by up to 1000 g·m⁻³ and by a factor of maximum 1.4, respectively employing the Takács-model. As a result of predicting higher biomass retention in the system, compared to simulation results obtained using the convection-dispersion SST model, values of the effluent NH₄N concentration predicted using the first-order model are lower by maximum 10 mg·L⁻¹ N and thus the effluent total N by maximum 6 mg·L⁻¹. Using the first-order model, as a result of the limited efficiency in predicting the SBH and thus the sludge inventory in the SST (see Fig. 3), the approximation of SRT is severely compromised, in most of the SVI range covered. According to the SRT data, shown in Fig. 4, for SVI<150 ml·g⁻¹, results obtained show approximately 4-day overestimation. This impact, for example, can also significant influence simulation efficiency – or the additional assumptions made by modellers – carried out using reactive settler models (also implemented in sequenced batch reactor models).



Figure 4 | Values of the relative $X_{TSS,In}$, effluent NH_{3,4}N, NO₃N, TN and SRT obtained using the two secondary settler models in the BSM1. Simulation results were obtained using BSM1 with the default model parameter set (defined at 15 °C) and with parameter values calculated at T=12 and 20 °C according to Melcer (2003).

For 150<SVI<200 ml·g⁻¹, between day 42 and 84, as a result of the ineffective estimation of sludge mass in the SST using the Takács-model, significantly more sludge is predicted to be washed-out from the system than that approximated using the convection-dispersion model. In effect, after day

84, with well-settling sludge in the SST (50<SVI<100), a significantly lower sludge mass and thus lower X_{TSS,In} concentration in the biological system is resulted with the WWTP model employing the Takács-sub-model.

We additionally assessed the simulation performance with liquid temperatures 12 and 20 °C. At 12 °C, the predicted severe wash-out of X_{AUT} from the system, predicted by the Plósz-model in days 42-84, causes a very high effluent NH₄N concentration that is maximum 18 mg·L⁻¹ N higher than that predicted by the Takács-model. Using the Plósz-model, the nitrification capacity is shown not to recover even under improving settling behaviour in days 70-84. Total N concentration values obtained suggest that, at high SVIs and at low liquid temperatures, the assessment of effluent concentration values can be under predicted by maximum 8 mg \cdot L⁻¹ N using the Takács-model. Simulation results obtained at 20 °C liquid temperature suggest that, in days 56-84, compared to simulation results obtained using the Plósz-model, the solids inventory in the bioreactors can also be significantly overestimated by the Takács-model. Following the day 84, X_{TSS,In} values obtained are comparable to that obtained using the BSM1 parameter set, whereas X_{AUT} concentrations are overestimated for another 14 days. Simulation results obtained at T=20 °C show that, although the 1-D SST model selection can significantly impact the prediction of solids inventory in the system, it does not have a such a severe effect on the approximation of the biological nitrogen removal as, for instance, in winter operation. This can be explained by that the X_{AUT} wash-out can be mitigated by higher autotrophic microbial growth rates. We note that the BSM1 is defined at 15 °C that can explain why the results are obtained in between the two other simulations.

CONCLUDING REMARKS

In WWTP simulations, using only default settling velocity function parameters is unsatisfactory, and can potentially deteriorate the overall simulation performance. A relatively simple engineering solution can be the monitoring of DSVI and the use of correlation factors and equations to calculate settling velocity function parameters in the model. Caution should; however, be exercised when using these correlations for their theoretical background is unclear.

According to the measured and numerical experimental as well as literature data, results obtained in the scenario analysis and WWTP modelling suggest that one of the convection-dispersion models, assessed in this study, is superior to the Takács-model in describing the SST. We therefore strongly advocate the use of the convection-dispersion model for use in WWTP simulations. This conclusion can be supported by the following remarks:

- For the secondary clarifier, the 1-D model realism can be considerably improved, in terms of (i) sludge blanket height under moderate and high sludge loading conditions; (ii) sludge concentration in the sludge recirculation stream under high and critical loading conditions; and (iii) effluent solids concentration under all loading conditions.
- For a range of 50 to 200 ml·g⁻¹ SVI, simulation results obtained using the BSM1 suggest that the predicted solids retention time can be severely overestimated and thus the biological nitrogen removal potential underestimated using the Takács sub-model. These negative impacts on the simulation performance can be further increased when deteriorated sludge settling behaviour is coupled with low liquid temperatures a typical scenario in real systems in winter periods.

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