

## Shall we upgrade one-dimensional secondary settler models used in WWTP simulators? – An assessment of model structure uncertainty and its propagation

Benedek Gy. Plósz, Jeriffa De Clercq, Ingmar Nopens, Lorenzo Benedetti and Peter A. Vanrolleghem

### ABSTRACT

In WWTP models, the accurate assessment of solids inventory in bioreactors equipped with solid-liquid separators, mostly described using one-dimensional (1-D) secondary settling tank (SST) models, is the most fundamental requirement of any calibration procedure. Scientific knowledge on characterising particulate organics in wastewater and on bacteria growth is well-established, whereas 1-D SST models and their impact on biomass concentration predictions are still poorly understood. A rigorous assessment of two 1-DSST models is thus presented: one based on hyperbolic (the widely used Takács-model) and one based on parabolic (the more recently presented Plósz-model) partial differential equations. The former model, using numerical approximation to yield realistic behaviour, is currently the most widely used by wastewater treatment process modellers. The latter is a convection-dispersion model that is solved in a numerically sound way. First, the explicit dispersion in the convection-dispersion model and the numerical dispersion for both SST models are calculated. Second, simulation results of effluent suspended solids concentration ( $X_{TSS, Eff}$ ), sludge recirculation stream ( $X_{TSS, RAS}$ ) and sludge blanket height (SBH) are used to demonstrate the distinct behaviour of the models. A thorough scenario analysis is carried out using SST feed flow rate, solids concentration, and overflow rate as degrees of freedom, spanning a broad loading spectrum. A comparison between the measurements and the simulation results demonstrates a considerably improved 1-D model realism using the convection-dispersion model in terms of SBH,  $X_{TSS, RAS}$  and  $X_{TSS, Eff}$ . Third, to assess the propagation of uncertainty derived from settler model structure to the biokinetic model, the impact of the SST model as sub-model in a plant-wide model on the general model performance is evaluated. A long-term simulation of a bulking event is conducted that spans temperature evolution throughout a summer/winter sequence. The model prediction in terms of nitrogen removal, solids inventory in the bioreactors and solids retention time as a function of the solids settling behaviour is investigated. It is found that the settler behaviour, simulated by the hyperbolic model, can introduce significant errors into the approximation of the solids retention time and thus solids inventory of the system. We demonstrate that these impacts can potentially cause deterioration of the predictive power of the biokinetic model, evidenced by an evaluation of the system's nitrogen removal efficiency. The convection-dispersion model exhibits superior behaviour, and the use of this type of model thus is highly recommended, especially bearing in mind future challenges, e.g., the explicit representation of uncertainty in WWTP models.

**Key words** | activated sludge, convection-dispersion model, numerical approximation, one-dimensional modelling, secondary settling tank, solids settling parameters, WWTP modelling

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## INTRODUCTION

In WWTP simulation environments, biological process models are mostly combined with one-dimensional secondary settler models (1-D SST) mainly for restricting computational burden. However, a 1-D model of the settler is inherently a simplification of the real system and of the underlying processes and conditions (e.g., gravity and compression settling, viscosity, dispersion, upward and downward convection, turbulence, buoyancy, inlet/outlet structure, sludge collection mechanisms) prevailing in a three-dimensional reactor. Hence, in order to obtain an effective simulation performance in 1-D, it is crucial that the SST model accounts for some of the important fluid dynamic processes and boundary conditions. The 1-D SST model identification/calibration is not a trivial process, and it requires sound mathematical solutions and high quality experimental observations. To simulate the detailed hydrodynamics of SSTs, 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 for plant-wide model applications. 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 De Clercq (2003). In order to implement this method for the first time, Plósz *et al.* (2007) used CFD simulation results, obtained with the Weiss model, to develop a 1-D SST model. Using this model, an accurate approximation of the solids profile in a flat-bottom SST could be achieved, thereby also improving the prediction of  $X_{TSS,EF}$  concentration and solids thickening under a broad range of flow conditions, including critical overloading (Plósz *et al.* 2007).

First-order 1-D SST models are based on a governing equation that includes convective “bulk” movement ( $U$ ) and gravity sedimentation ( $v_s$ ) on a small section of height  $\delta z$ , leading to the hyperbolic continuity equation:

$$-\frac{\partial X_{TSS}}{\partial t} = U \frac{\partial X_{TSS}}{\partial z} + \frac{\partial (v_s X_{TSS})}{\partial z}, \quad (1)$$

where the solids concentration,  $X_{TSS}$ , is dependent on the time ( $t$ ) and on the spatial coordinate ( $z$ ). We note that Equation (1) does not include any inlet source or outlet sink terms. These are dealt with through appropriate boundary conditions. A drawback of this model is the fact that the solids concentration depends only on the height of the layer ( $z$ ), and not on the concentration gradient. With regard to models based on Equation (1), the most well-known is the

one developed by Takács *et al.* (1991), also including the widely used double-exponential gravity settling function. In this landmark work, using the finite difference approximation, the “rough” discretisation (10 layers) of this first-order model introduces significant numerical dispersion that effectively contributes to finding a smooth concentration profile, representative of typically observed sludge concentration profiles (Takács 2008). For a range of clarifier depths, the correlation of this numerical dispersion with convective velocities above/below the fixed feed-layer can result in effective model performance, as evidenced by ample literature of successful application. However, a drawback of this approach is the lack of control over the dispersion term that confines the validity of a best fit calibration to a limited range of flow and concentration boundary conditions. Indeed, as Krebs (1995) noted, it is possible to find a best fit calibration for almost any set-up, and an inappropriate layer arrangement can be compensated for by unrealistic parameter calibration of the settling properties.

The numerical dispersion introduced in finite difference approximations can be quantified based on the analytical solution obtained for the variance ( $\sigma^2$ ) of the probability density for the residence time ( $\tau$ ) in the reactor/clarifier closed for turbulence (e.g., Gujer 2008),

$$\frac{\sigma^2}{\tau_m^2} = \frac{1}{n} = 2 \cdot N_T - 2 \cdot N_T^2 \cdot \left[ 1 - \exp\left(-\frac{1}{N_T}\right) \right], \quad (2)$$

where  $\tau_m$  and  $n$  denote the mean hydraulic residence time and the number of vertical, completely mixed clarifier segments (1-D model layers), respectively. A system is closed for turbulence when convection dominates in the influent and effluent, and turbulence is confined to the reactor volume. Here  $N_T$  is the numerical dispersion number (dimensionless), written as

$$N_T = \frac{D_T}{U \cdot \delta z} \quad (3)$$

that characterises the numerical dispersion,  $D_T/\delta z$ , relative to the convective velocities ( $U$ ) in the clarifier underflow and overflow region.

For  $N_T \ll 1$ , based on Gujer (2008), the  $D_T/\delta z$  value can then be approximated using

$$\frac{D_T}{\delta z} = \frac{U}{2 \cdot n}. \quad (4)$$

We note that, using finite difference methods to solve partial differential equations (PDEs), numerical dispersion is

additionally impacted by the time step size ( $\delta t$ ) selected for integration. Despite the progress made in the last two decades in the field (Watts *et al.* 1996; Diehl & Jeppsson 1998; Bürger *et al.* 2005; Plósz *et al.* 2007; De Clercq *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 fact that most of the software packages provide only the Takács model, and that WWTP process modellers either ignore the settler performance in their assessment studies or may not be aware of the development in the field. 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,

$$-\frac{\partial X_{TSS}}{\partial t} = U \frac{\partial X_{TSS}}{\partial z} + \frac{\partial(v_s X_{TSS})}{\partial z} - D_C \frac{\partial^2 X_{TSS}}{\partial z^2}, \quad (5)$$

representing a parabolic PDE. The second order derivative term allows accounting for compression settling and/or solid dispersion. The latter process can be characterised by an explicit dispersion coefficient ( $D_C$ ) that is a characteristic of 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 SST 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. Furthermore, the introduction of the dispersion term helps to distinguish between effects of sludge settleability and other effects, e.g., sludge removal (Ekama *et al.* 1997).

The question arises how the model selection for representing the SST in an integrated wastewater treatment plant (WWTP) model does influence the overall simulation performance of the model, including the interaction between the bioprocess model and the settler model. Hence, the paper does not limit itself to comparing two settler models, but extends the investigation to the plant-wide model level, i.e., what are the effects of the choice of the settler model on other WWTP model predictions such as nutrient removal? In order to assess the behaviour of both 1-D SST models, we rely on experimental data (De Clercq 2006) and on numerical validated observations presented in literature (Plósz *et al.* 2007).

The principal aim of the present work is to perform a rigorous comparison of the commonly used Takács model and a convection-dispersion settler model (Plósz *et al.* 2007) that is similar to that developed by De Clercq *et al.* (2008). In the first part, values of the explicit dispersion in the convection-dispersion model and the numerical dispersion for both SST models are assessed. In the second part, a scenario

analysis using the Takács and the Plósz 1-D SST models is performed using ranges of SST feed, underflow rate and feed solids concentrations as degrees of freedom. Moreover, results are compared with measured data. In the third part, the impact of both 1-D SST models used as sub-models in a dynamic WWTP model on the simulation results is investigated. Impacts of a time-varying SSVI<sub>3,5</sub> series that is translated into settling velocity function parameters through a correlation (to mimic a bulking event) as well as the effects of temperature are investigated.

## MATERIALS AND METHODS

### Continuous settling experiments

Full-scale experiments were carried out in two different SSTs, those of the Heist and Essen WWTPs (Belgium). Sludge blanket heights were measured every 10 min with a Staiger-Mohilo 7210 MTS probe. The minimum concentration in the sludge blanket defined was 0.8 kg m<sup>-3</sup>. Solids concentration in the effluent and in the recycle flow was measured every 4 h according to *Standard Methods* (1995). For more information on the experiments, the reader is referred to De Clercq (2006).

### Batch settling experiments

Batch settling curves were measured using a SettleMeter (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<sup>®</sup> (MOSTfor-WATER NV, Kortrijk, 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), further referred to as the first-order model, and that by Plósz *et al.* (2007), further referred to as the 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 ( $v_0$ ), 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 Benchmark Simulation Model Nr. 1, BSM1 (Copp *et al.* 2002). In any given layer with solid concentration above an arbitrary threshold, typically  $X_T = 3 \text{ kg}\cdot\text{m}^{-3}$ , to avoid higher concentration in the adjacent upper layer, a minimum settling flux condition is set.

### 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).

The Gujer matrix, also known as the Petersen matrix, is often used to represent activated sludge models, in which 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  $\Delta t$ , density currents are taken into account by positioning the feed layer  $i = f$  above the first layer that has a concentration larger 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 profiles 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.

Furthermore, the 1-D SST model includes a feedflow-dependent reduction factor in the downward convection term ( $\eta_C$ ), and the dispersion coefficient is governed as a function of the clarifier overflow velocity. Minimum settling flux conditions are formulated above and below the feed layer using the Godunov scheme that was proven correct by Diehl & Jeppsson (1998). We note that De Clercq *et al.* (2008) used the Engquist-Osher flux that was proven correct by Bürger *et al.* (2005). The fourth-order Runge-Kutta (RK4ASC) 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. Using the first-order and the convection-dispersion model, for the 126-day dynamic simulations, the computation times required (Processor: IntelCore-i7, 2.67 GHz) were 1.26 and 3.19 min, respectively. This result is particularly convincing, considering that, in BSM1, the SST model accounts for a significant part of the overall model, which is not the case for typical WWTP models, e.g., BSM2 (Jeppsson *et al.* 2007). In general, thus, the difference in computational time is expected to be smaller.

### Scenario simulations

Scenarios were simulated in a case study using a SST with a horizontal surface area,  $A_{SST} = 1,000 \text{ m}^2$  and vertical depth,  $H_{SST} = 3 \text{ m}$ . 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.

For the simulations, the settling model parameters used are presented by Plósz *et al.* (2007):  $v_0 = 100.5 \text{ m d}^{-1}$ ;  $r_H = 0.287 \text{ m}^3 \text{ kg}^{-1}$ ;  $r_P = 10 \text{ m}^3 \text{ kg}^{-1}$ ;  $f_{NS} = 0.00138$ ;  $D_{C,0} = 3.95 \text{ m}^2 \text{ d}^{-1}$ ;  $\gamma = 2.210 \cdot 10^{-2} \text{ d}$ ;  $v_{Ov,C} = 15 \text{ m d}^{-1}$ ;  $\eta_{C,0} = 0.5$ ;  $v_{F,C} = 30.5 \text{ m d}^{-1}$ .

### WWTP modelling

In addition to a mere comparison of both models, we also assessed the behaviour and realism of the models as part of

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

Clarifier grid points	$i=1$	$1 < i < f$	$i=f$	$f < i < sc$	$sc \leq i < n$	$i=n$	Rate equations
Solids fluxes, $(\frac{dC_i}{dz}) \downarrow$	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	
1. Gravity settling	$-v_{S,i}C_i$	$v_{S,i-1}C_{i-1} - v_{S,i}C_i$				$v_{S,i-1} \cdot C_{i-1}$	$v_{S,i} = v_0 \left( e^{-\eta_i(C_i - f_{SS}C_f)} - e^{-\eta_i(C_i - f_{SS}C_f)} \right)$
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
							$\eta_C = \begin{cases} \eta_{C,0} & \text{if } v_F < v_{FC} \\ \min \left\{ \eta_{C,0} + \left( \frac{v_F - v_{FC}}{v_{FC}} \right)^2 ; 1 \right\} & \text{if } v_F \geq v_{FC} \end{cases}$
4. Solids dispersion	$D_{C,i}(C_{i+1} - C_i)$						$D_{C,i} = \frac{D_C}{\delta z},$ where
							$D_C = \begin{cases} D_{C,0} & \text{if } v_{Ov} < v_{Ov,C} \\ D_{C,0} + \gamma(v_{Ov} - v_{Ov,C})^2 & \text{if } v_{Ov} \geq v_{Ov,C} \end{cases}$
5. Clarifier inflows and outflows	$-v_{Ov}C_i$		$v_F C_f$		$-v_{Un,i}C_i$		$v_{Ov} = \frac{Q_{Over}}{A_{SST}} \quad v_F = \frac{Q_{Feed}}{A_{SST}} \quad v_{Un,i} = \frac{Q_{Under,i}}{A_{SST}},$ and
							$Q_{Under} = \sum_{i=SC}^n Q_{Under,i}$

**Table 2** | Boundary conditions used in the scenario analysis

$Q_{\text{Feed}}$ ( $\text{m}^3 \cdot \text{d}$ )	$Q_{\text{Under}}$ ( $\text{m}^3 \cdot \text{d}$ )	$X_{\text{TSS,Feed}}$ ( $\text{kg} \cdot \text{m}^{-3}$ )
20,000	10,000	2.2
35,000	15,000	3
45,000	20,000	4
51,000	25,000	4.5

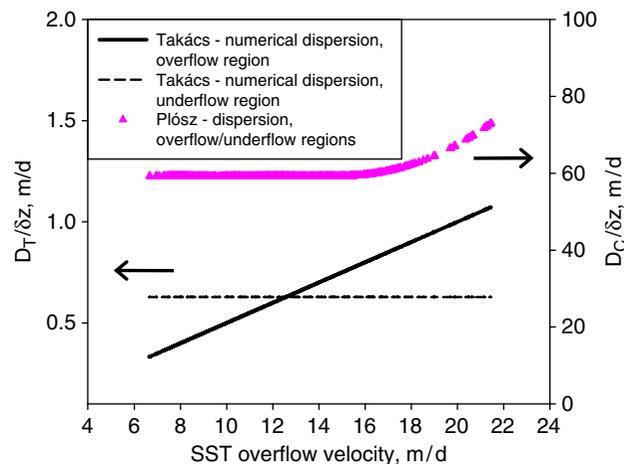
the pre-anoxic-aerobic activated sludge system ( $A_{\text{SST}}=1,500 \text{ m}^2$ ;  $H_{\text{SST}}=4 \text{ m}$ ;  $Q_{\text{Under}}=18,831 \text{ m}^3 \cdot \text{d}^{-1}$ ;  $Q_{\text{Wastage}}=385 \text{ m}^3 \cdot \text{d}^{-1}$ ;  $Q_{\text{Nitrat}}=55,338 \text{ m}^3 \cdot \text{d}^{-1}$ ) 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- ( $Q_{\text{Nitrat}}$ ) and sludge-recirculation streams ( $Q_{\text{Under}}$ ), and excess sludge removal ( $Q_{\text{Wastage}}$ ) 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 ( $K_L a$ ) of  $240 \text{ d}^{-1}$ ,  $240 \text{ d}^{-1}$  and  $84 \text{ d}^{-1}$ . 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.,  $K_L a=0$ . 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 for the WWTP simulation is based on the BSM1. 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, which may well be a significant factor, influencing the overall solids settling.

## RESULTS AND DISCUSSION

### Dispersion and numerical dispersion in the SST models

In order to solve Equations (1) and (5), the difference schemes used in the discretisation of the Takács and the Plósz model include 10 and 60 layers, respectively. For the overflow and underflow boundary conditions set in the BSM1, values of the numerical dispersion created by the Takács model in the overflow region ( $(D_T/\delta z)_{Ov}$ ) were calculated using Equation (4), and are shown in Figure 1.

For the underflow region the  $(D_T/\delta z)_{Un}$  value calculated is  $0.63 \cdot \text{d}^{-1}$  (constant recycle flow velocity) (Figure 1,



**Figure 1** | Values of the numerical dispersion ( $D_T$ ) induced by the Takács model (left axis) and of the explicit dispersion ( $D_C$ ) employed in the Plósz model (right axis) plotted as a function of the SST overflow velocity.

dashed line). We note that, in the Takács model, the *ad hoc* minimum settling flux condition does not only prevent inverse gradients but also acts as a kind of concentration-dependent dispersion coefficient, thereby increasing the overall dispersion. Compared to numerical dispersion, this dispersion can be significant using 10 layers; however, we did not explicitly assess it, mainly because it changes from layer to layer as a function of the concentration difference. For  $\delta z \rightarrow 0$ , similarly to the numerical dispersion, the impact of minimum settling flux condition becomes negligible, thereby causing the model prediction to deteriorate at finer discretisations (Watts et al. 1996), e.g., using 60 layers. In other words, for the Takács model, if a higher discretisation level had been chosen than the widely used 10-layer, then model realism would have been negatively affected. It is noteworthy that the impact of the time step size ( $\delta t$ ) on numerical dispersion was not accounted for in our calculation. One of the reasons for that is that the RK4ASC integrating method employs a variable  $\delta t$  value (minimum value used in this study:  $0.0001 \text{ d}$ ) whose adequacy is verified at each time step. This protects against numerical errors. Based on Equation (4), the numerical dispersion created by the Plósz model is six times lower than that in the Takács model. In Figure 1, we additionally show the explicit dispersion,  $D_C/\delta z$ , values calculated for the Plósz-model (for the calculation of  $D_C$ , see Table 1;  $\delta z=4/60 \text{ m}$ ,  $v_{Ov,C}=15 \text{ m d}^{-1}$ ) that are thus over 650 times higher than the numerical dispersion  $(D_T/\delta z)_{Ov}$  caused by the 60-layer discretisation. The latter is thus negligible, as it should be.

The results plotted in Figure 1 clearly show the difference between the numerical dispersion in the first-order model

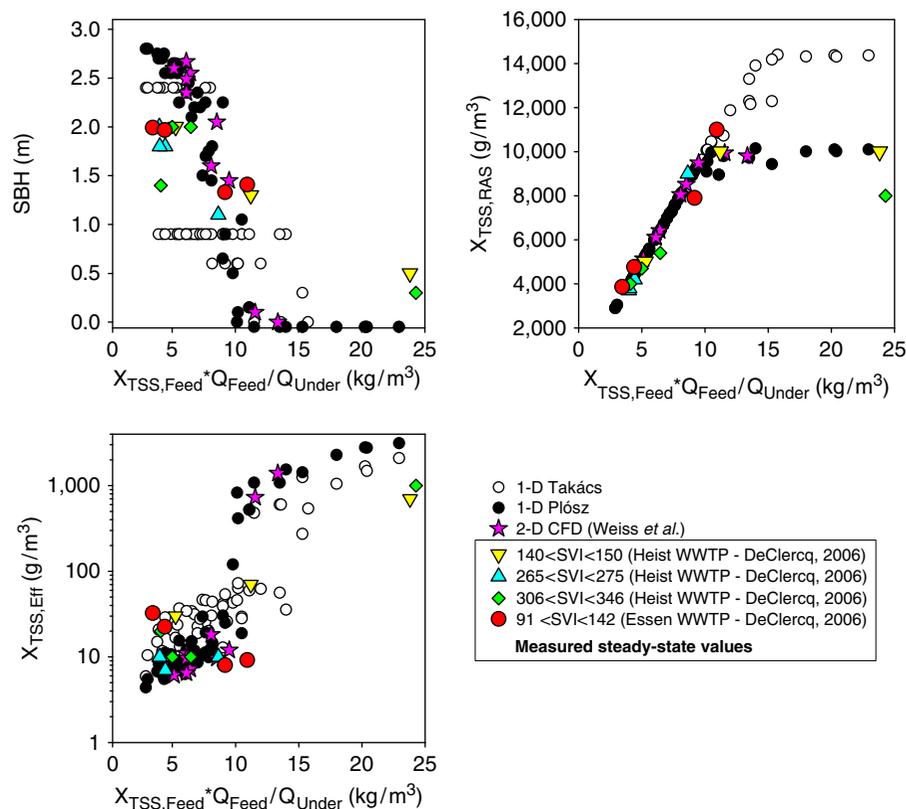
(approximately between 0.3 and 1.1 m·d<sup>-1</sup>) and the dispersion in the convection-dispersion model (59 to 74 m·d<sup>-1</sup>). This impact can potentially lead to different model predictions under a wide range of flow boundary conditions, as will be discussed below. It can also be a potential source of deterioration in the predictive power in the Takács model, in which (numerical) dispersion cannot be explicitly calibrated as a function of flow.

## Scenario simulations

In Figure 2, the 1-D and 2-D CFD simulation results as well as measured experimental data are compared for sludge blanket height (SBH), total suspended solids concentration in the recirculation stream ( $X_{TSS,RAS}$ ) and in the clarifier overflow ( $X_{TSS,EF}$ ). The results obtained are plotted as a function of SST mass-loading normalised to the underflow rate,  $\varphi = X_{TSS,Feed} \cdot Q_{Feed} / Q_{Under}$ . At  $\varphi$  values below 10 kg m<sup>-3</sup>, 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 seven times higher  $X_{TSS,EF}$ . For  $10 \leq \varphi \leq 20$  kg m<sup>-3</sup>, simulation results obtained with the Takács model show (i) 1 to 1.5 times higher  $X_{TSS,RAS}$ , (ii) 0.06 to 0.67 times lower  $X_{TSS,EF}$ , and (iii) 0.68 to 0.98 times lower SBH values than those obtained with the Plósz model. Within the  $2.2 \leq \varphi \leq 25$  kg·m<sup>-3</sup> interval, increasing SBH values can be observed along with increasing  $X_{TSS,EF}$  using the Plósz model. Ekama et al. (1997) demonstrate using measured data that higher sludge blanket heights translate to higher effluent suspended solids. Effluent total suspended solids concentration values ( $X_{TSS,EF}$ ) obtained using the Plósz model show a breakthrough, i.e., sludge washout event, characterised by an inflection point at  $\varphi = 10$  kg·m<sup>-3</sup>.

For  $X_{TSS,EF}$  values, results obtained with the Takács model indicate a diffuse transition from  $\varphi = 2$  to 15 kg·m<sup>-3</sup> without showing any breakthrough. A striking thing about the SBH obtained with the Takács model is that, for  $2.2 \leq \varphi \leq 10$  kg m<sup>-3</sup>, its value oscillates between 0.6 and 2.1 m irrespective



**Figure 2** | 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 ( $X_{TSS,EF}$ ). Note that, to compare data derived from different SSTs, here SBH = 0 is at the liquid surface, i.e. it shows the depth of the sludge blanket. The scenario analysis was carried out using the two 1-D SST models for a hypothetical SST ( $A_{SST} = 1000$  m<sup>2</sup>;  $H_{SST} = 3$  m). Steady-state CFD simulation results were obtained for a flat-bottom SST ( $A_{SST} = 855$  m<sup>2</sup>;  $H_{SST} = 3$  m). Measured values were obtained in two conical SSTs (Heist:  $A_{SST} = 254$  m<sup>2</sup>;  $H_{SST, side-wall} = 1.92$  m;  $H_{SST, centre} = 2.41$  m; Essen:  $A_{SST} = 292$  m<sup>2</sup>;  $H_{SST, side-wall} = 1.88$  m;  $H_{SST, centre} = 2.56$  m).

of the loading conditions applied in the scenario analysis. This factor can introduce significant uncertainties in calculating the sludge inventory in the SST, as shown in the subsequent section of this paper. Values of  $X_{TSS,RAS}$  obtained with the Takács model, plotted at  $\varphi > 10 \text{ kg m}^{-3}$ , suggest an overestimation of solids thickening, and thus very high concentration levels in the recycle stream (see below for a discussion on the effect this has on the bioreactor behaviour). We attribute this model behaviour, in part, to the impact of the concentration-dependent dispersion introduced by the minimum settling flux condition in the Takács model. Using the convection-dispersion model, such model structure uncertainty can effectively be avoided.

Under critical loading conditions, i.e., at  $\varphi > 10 \text{ kg m}^{-3}$ , simulation results obtained for  $X_{TSS,EFF}$  using the Takács model are significantly lower than those obtained with the Plósz model. Under moderate and low loading, i.e., at  $\varphi < 10 \text{ kg m}^{-3}$ , Parker *et al.* (2001) show that proper activated sludge system operation with good SST design results in average  $X_{TSS,EFF}$  around  $10 \text{ g m}^{-3}$ .  $X_{TSS,EFF}$  values obtained with the Takács model at  $\varphi < 10 \text{ kg m}^{-3}$  thus suggest an overestimation of a properly designed and functioning SST effluent quality. This is not the case for the Plósz model. For  $5.13 < \varphi < 13.4 \text{ kg m}^{-3}$ , Plósz *et al.* (2007) investigated the performance of an SST ( $A_{SST} = 855 \text{ m}^2$ ;  $H_{SST} = 3 \text{ m}$ ) using the 2-D CFD model by Weiss *et al.* (2007), evaluated and confirmed using measured data. In Figure 2, seven 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  $3.45 < \varphi < 24.3 \text{ kg m}^{-3}$ , De Clercq (2006) presented steady-state data measured in two conical SSTs (characteristics shown in Figure 2). We note that, for the 1-D scenario simulations, we only used one set of settling velocity parameters, whereas the measured data were obtained for a wide range of SVIs. Also, to compare data derived from different SSTs, for Figure 2,  $SBH = 0$  is defined at the liquid surface, i.e., SBH shows in fact the depth of the sludge blanket. At  $\varphi < 6.5 \text{ kg m}^{-3}$ , the measured SBH values are significantly lower than the 1-D simulation results obtained using the convection-dispersion model, and they are around 1.9 m distant from the liquid surface that is approximately equal to the side-wall depths of these SSTs. The main reason for this discrepancy is that the two conical SSTs have a 0.5–1m shallower centre-depth than the other flat bottom clarifiers studied. Parker *et al.* (2001) show that, in a conical SST compared to a flat-bottom reactor, higher sludge blankets can develop because of (i) the development of the compres-

sive blanket beginning from a higher elevation; (ii) sludge conveyance inefficiencies; (iii) less storage volume for the same depth in the centre.

At  $\varphi < 6.5 \text{ kg m}^{-3}$ , for reasonably well settling sludge, i.e.,  $SVI < 150 \text{ mL g}^{-1}$ , measured  $X_{TSS,RAS}$  and  $X_{TSS,EFF}$  data show a close agreement with the simulation results obtained with the Plósz model. For  $6.5 < \varphi < 13.5 \text{ kg m}^{-3}$ , 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 overloading,  $\varphi \sim 24 \text{ kg m}^{-3}$ , the measured SBH is somewhat lower than the model approximation, which can, in part, explain the lower  $X_{TSS,EFF}$  value simulated with the 1-D SST models. 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. In general, for properly designed/functioning SSTs and for  $SVI < 150 \text{ mL g}^{-1}$ , the  $X_{TSS,EFF}$  prediction can thus be limited under SST overloading conditions, and is a matter of case-specific, forced calibration. For  $SVI < 150 \text{ mL g}^{-1}$ , despite the different geometrical characteristics of the SSTs considered, the simulated (Plósz model) and measured  $X_{TSS,RAS}$  results (two identical values at  $\varphi = 24 \text{ kg m}^{-3}$ ) agree well. We note, however, that in this concentration range the reliability of the sensor used in the study was relatively weak, i.e., the concentration may have been higher.

It is noteworthy that, at  $6 < \varphi < 25 \text{ kg m}^{-3}$ , despite the different SST geometries considered and sludge settling properties, simulation results obtained using the Plósz model for the SBH,  $X_{TSS,RAS}$  and  $X_{TSS,EFF}$  agree fairly well with the measured data. In steady state, mass balance dictates that the sum of the effluent  $X_{TSS,RAS}v_{Ov}$  and  $X_{TSS,EFF}v_{Uf}$  fluxes must equal the input  $X_{TSS,Feed}v_F$  flux. According to Figure 2, for low  $X_{TSS,EFF}$  values, i.e., below  $80 \text{ g m}^{-3}$ , the calculation of the  $X_{TSS,RAS}v_{Ov}$  mass flux is not significantly impacted by the overprediction of the  $X_{TSS,EFF}$  using the Takács model. This, however, is not the case for  $X_{TSS,EFF}$  values above  $80 \text{ g m}^{-3}$ . Compared to measured data and simulation results obtained with the Plósz model, the underprediction of the  $X_{TSS,EFF}$  and the overprediction of the solids' thickening behaviour, obtained using the Takács model, results in a significantly increased mass-flux recycled into the bioreactors. Since the settling velocity function parameters are the same for both models (except for the maximum practical settling velocity parameter that is omitted in the Plósz model), the discrepancy between the 1-D simulation results is mainly caused by the different ways the two models and their numerical integration assess dispersion in the SST. The assessment of model behaviour under dynamic conditions can potentially reveal further

advantages/drawbacks of 1-D mathematical descriptions of the settler – an exercise that will be presented in a forthcoming paper.

## WWTP modelling

A long-term simulation study, including normal operation, followed by a bulking event and subsequently improving sludge settleability, has been performed under dry- and wet-weather conditions.

## Relationships between sludge settleability parameters

To implement the time-varying settling properties defined in terms of a SSVI sequence, a correlation had first to be established between SSVI<sub>3,5</sub> data and settling velocity function parameters. The stirred specific volume index (SSVI<sub>3,5</sub>) 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 mL·g<sup>-1</sup> (Figure 3). 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). Values obtained for  $v_0$  and  $r_H$  are correlated with the SSVI<sub>3,5</sub> using the general equations by Ekama et al. (1997). Data obtained indicate the temperature dependence of  $v_0$  and  $r_H$ ; however, due to the lack of data, it is not possible for us to evaluate a different set of parameters at higher temperatures. We have found values of 133.7 m d<sup>-1</sup> and 3.4 kg m<sup>-3</sup> for  $\alpha$  and  $\beta$ , respectively.

$$v_0 = \alpha \exp(-\beta \times \text{SSVI}_{3,5}) \quad (R^2 = 0.02) \quad (6)$$

$$r_H = \kappa + \lambda \times \text{SSVI}_{3,5} \quad (R^2 = 0.78) \quad (7)$$

The correlation for  $v_0$  shows that this parameter is practically independent of the SSVI<sub>3,5</sub>, and  $v_0 \sim \alpha$ . Values obtained for  $\lambda$  and  $\kappa$  are 0.0026 m<sup>3</sup>·L<sup>-1</sup> and 0.0628 m<sup>3</sup>·kg<sup>-1</sup>, respectively. These results are in close agreement with the data reported by Ekama et al. (1997). In the authors' opinion, however, such correlations should be used with care, for their theoretical background is unclear – see, e.g., Dick & Vesilind (1969) and the presence of outlier data (based on visual observation) in Figure 3.

## SST 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<sup>-1</sup>, using the correlations Equations (6) and (7). We note that, in our simulation model, compared to the default settings in BSM1, the  $r_P$  and  $f_{NS}$  parameter values are changed to 10 m<sup>3</sup>·kg<sup>-1</sup> and 0.00138, respectively, as suggested by Plósz et al. (2007). A sequence of the default input-time series, i.e., nine times the 14 days of influent data, is combined with DSVI values set for each 14-day period. In Figure 4, values of SBH,  $X_{TSS,RAS}$  and  $X_{TSS,EF}$  obtained are plotted as a function of the time elapsed and of the DSVI. We note that, for Figure 4 and Figure 5, in contrast to Figure 2, SBH=0 is defined at the SST bottom. As a function of the progressively deteriorating sludge quality (days 0–42), the Takács model shows a “fuzzy” prediction of the SBH (Figure 4a) – an impact that can cause severe deterioration in the assessment of sludge retention time (SRT) in the system (see Figure 5). This is not the case for the Plósz model, which suggests a gradually increasing, i.e., more realistic, blanket depth. For SVI=150 and 200 mL g<sup>-1</sup> (days 43–70), sludge thickening deteriorates, thereby also decreasing  $X_{TSS,RAS}$  values (Figure 4b). Using the Plósz model, simulation results suggest approximately 1,000 and

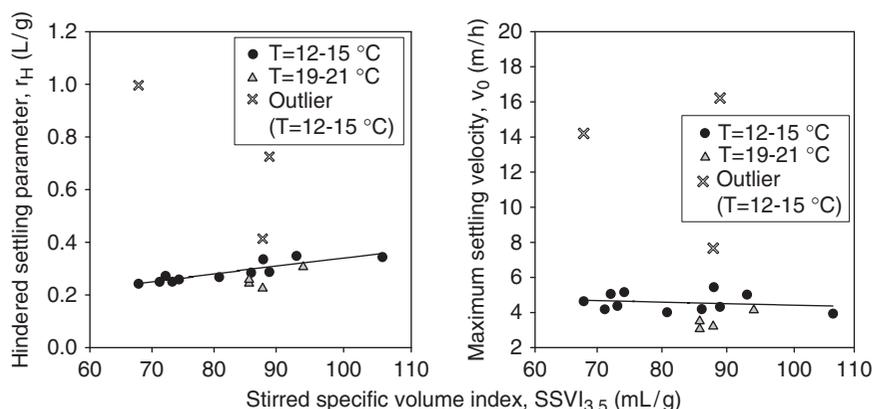
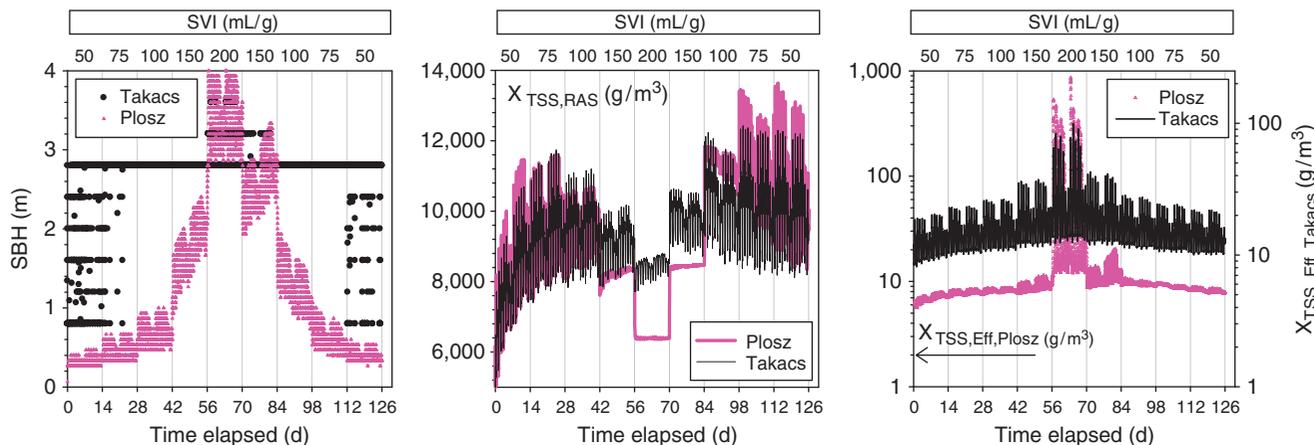


Figure 3 | Values of hindered settling parameter (A – left) and the maximum settling velocity (B – right) plotted as a function of stirred specific volume index.



**Figure 4** | Values of the sludge blanket height (A – left),  $X_{TSS,RAS}$  (B – middle) and  $X_{TSS,Eff}$  (C – right) obtained with the BSM1.

1,500  $\text{g m}^{-3}$  lower  $X_{TSS,RAS}$  values on average than the Takács model.

For  $50 \leq \text{SVI} \leq 150 \text{ mL g}^{-1}$ , values of  $X_{TSS,Eff}$  are between 15 and 80  $\text{g m}^{-3}$  (Figure 4c), which are significantly higher than that simulated by the Plósz model. For  $50 \leq \text{SVI} \leq 100 \text{ mL g}^{-1}$ , according to Figure 4b,  $X_{TSS,RAS}$  values predicted by the two models do not deviate significantly. This is in good agreement with our observations made on steady-state data as to the impact of  $X_{TSS,Eff} < 80 \text{ g m}^{-3}$  on the calculation of the  $X_{TSS,RAS} \nu_{Ov}$  mass flux. In Figure 4c, between days 56 and 70, severe sludge washout is predicted by the Plósz model,  $X_{TSS,Eff}$  values up to 800  $\text{g m}^{-3}$ , which is not the case for the Takács model that predicts  $X_{TSS,Eff}$  values only up to 270  $\text{g m}^{-3}$ .

### Biological treatment performance

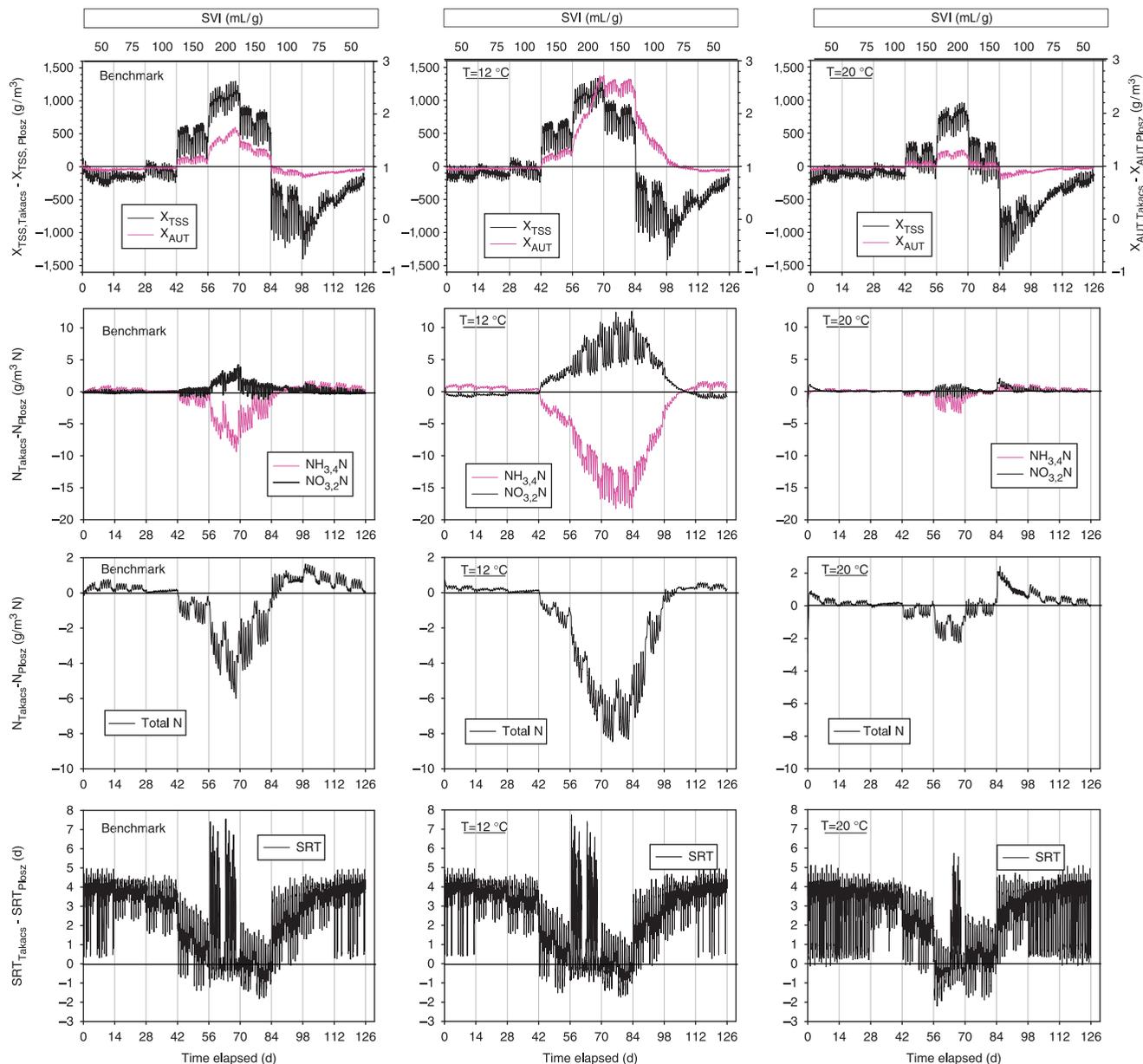
In Figure 5, the calculated differences between the simulation output regarding the bioreactor, obtained using the Takács and the Plósz model, are plotted. The selected state-variables are the total suspended solids concentration in the last aerobic reactor ( $X_{TSS,In}$ ), autotrophic biomass concentration ( $X_{AUT}$ ) 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  $\Delta t$ , 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) presents a method to calculate the dynamic SRT of activated sludge systems.

For the BSM1 parameter setting (left column in Figure 5), 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 1,000  $\text{g m}^{-3}$  and by a factor of maximum 1.4, respectively, employing the Takács model. For  $150 \leq \text{SVI} \leq 200 \text{ mL g}^{-1}$ , as a result of the over-prediction of the maximum retainable solid mass in the settler and the  $X_{TSS,RAS}$  (see Figure 4a and b), significantly longer biomass retention is predicted in the system (bioreactors + SST). Consequently, the predicted nitrification capacity is increased and values of the effluent  $\text{NH}_4\text{-N}$  concentration predicted using the first-order model are lower by maximum 10  $\text{mg L}^{-1}$  N and the effluent total N by maximum 6  $\text{mg L}^{-1}$ . Using the first-order model, the approximation of SRT is severely compromised in most of the SVI range covered. According to the SRT data, shown in Figure 5 (left column), for  $\text{SVI} < 150 \text{ mL g}^{-1}$ , results obtained show approximately a 4-day overestimation. This impact can significantly influence the prediction of microbial retention time in the system – or the additional assumptions made by modellers on biological reaction kinetics using reactive settler models (also implemented in sequenced batch reactor models).

For  $150 \leq \text{SVI} \leq 200 \text{ mL g}^{-1}$ , between days 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 ( $50 < \text{SVI} < 100 \text{ mL g}^{-1}$ ), a significantly lower sludge mass and thus lower  $X_{TSS,In}$  concentration is observed in the biological system when employing the Takács sub-model.

A faulty prediction of sludge inventory will severely impact the overall WWTP model calibration exercise as conversion rates will be wrongly assessed using a faulty settler description. Typically, this will result in calibrating



**Figure 5** | Values of the relative  $X_{TSS,In}$ , effluent  $NH_{3,4}N$ ,  $NO_{3,2}N$ , 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 (left column) and with parameter values calculated at  $T = 12^\circ C$  (middle column) and  $20^\circ C$  (right column) according to Melcer (2003).

kinetic model parameters by process modellers to correct for the impact of the erroneous SST-submodel prediction. Then, the calibrated model will possibly be able to predict the process behaviour effectively only under narrow intervals of flow and settling boundary conditions. Therefore, the predictive power of such a model is low, and is of limited use to test different scenarios for, e.g., improving process performance.

We additionally assessed the simulation performance with liquid temperatures 12 and 20°C. At 12°C (middle column in Figure 5), the severe washout of  $X_{AUT}$  from the system, predicted by the Plósz model in days 42–84, causes a

very high effluent  $NH_4N$  concentration that is maximum  $18 \text{ mg L}^{-1} \text{ N}$  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. After day 84,  $X_{TSS,In}$  values obtained are comparable to those obtained using the BSM1 parameter set, whereas  $X_{AUT}$  concentrations are overestimated for another 14 days. 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  $8 \text{ mg L}^{-1} \text{ N}$  using the Takács model.

Simulation results obtained at 20°C liquid temperature (right column in Figure 5) 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. Simulation results obtained at  $T = 20^\circ\text{C}$  (right column in Figure 5) also show that, although the 1-D SST model selection can significantly impact the prediction of the solids inventory in the system, it does not have such a severe effect on the approximation of the biological nitrogen removal as, for instance, in winter operation. This can be explained by the fact that the  $X_{\text{AUT}}$  washout can be mitigated by higher autotrophic microbial growth rates. For reactive settler models, however, the overestimation of the system's solids retention time by the Takács model can potentially introduce a significant error into the biokinetic model prediction even at  $T = 20^\circ\text{C}$  – an impact not explicitly assessed here. We note that the model parameters used in the BSM1 are defined at 15°C, which may explain why these data are in between the other simulation results obtained at  $T = 12$  and  $20^\circ\text{C}$ .

## CONCLUSIONS

According to literature, measured and the CFD numerical experimental data, results obtained in the scenario analysis and WWTP modelling suggest that convection-dispersion models, of which one was assessed in this study, are superior to the Takács model in describing the SST. Additionally, the second-order model can effectively decrease the level of uncertainty introduced by the improper SST model structure – an impact that is shown to propagate to the biokinetic model. 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 a range of loading boundary conditions, the dispersion values computed by the Takács and Plósz models show a significant difference and a negligible numerical dispersion for the Plósz model.
- In contrast to the explicit (flow-dependent) dispersion term used in the Plósz and De Clercq convection-dispersion models, in the Takács model it is not possible to control the dispersion term. Consequently, modellers using the Takács model should compensate for the resulting error at the expense of forced (re-)calibration using unrealistic settling model parameters, particularly for simulations run under wide ranges of flow boundary conditions.

- For the secondary clarifier, the 1-D model realism can be considerably improved using the Plósz model, 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 the range of 50 to 200  $\text{mL}\cdot\text{g}^{-1}$  SVI, simulation results obtained using the convection-dispersion model in BSM1 suggest that the correct prediction of the system's solids retention time can allow a more effective assessment of the biological nitrogen removal potential than with the Takács model.
- Using the Plósz model, the predictive power 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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