Quantifying the sources of uncertainty when calculating the limiting flux in secondary settling tanks using iCFD

Estelle Guyonvarch, Elham Ramin, Murat Kulahci and Benedek G. Plósz

ABSTRACT

Solids-flux theory (SFT) and state-point analysis (SPA) are used for the design, operation and control of secondary settling tanks (SSTs). The objectives of this study were to assess uncertainties, propagating from flow and solids loading boundary conditions as well as compression settling behaviour to the calculation of the limiting flux ($J_L$) and the limiting solids concentration ($X_L$). The interpreted computational fluid dynamics (iCFD) simulation model was used to predict one-dimensional local concentrations and limiting solids fluxes as a function of loading and design boundary conditions. A two-level fractional factorial design of experiments was used to infer the relative significance of factors unaccounted for in conventional SPA. To move away from using semi-arbitrary safety factors, a systematic approach was proposed to calculate the maximum SST capacity by employing a factor of 23% and a regression meta-model to correct values of $J_L$ and $X_L$, respectively – critical for abating hydraulic effects under wet-weather flow conditions.

Key words | computational fluid dynamics, interpreted computational fluid dynamics model (iCFD), one-dimensional advection dispersion model, secondary settling tank, solids-flux theory, statistical factor screening

GLOSSARY OF TERMS

Abbreviations

1D One dimensional
2D Two dimensional
2LFDE Two-level fractional factorial design of experiments
CFD Computational fluid dynamics
iCFD Interpreted computational fluid dynamics
LHS Latin hypercube sampling
RAS Return activated sludge
SBH Sludge blanket height
SF Safety factors
SFT Solids-flux theory

SPA State-point analysis
SHC Solids handling criteria
SSRE Sum of square of relative errors
SST Secondary settling tank
SWD Side water depth
TSS Total suspended solids
WWTP Wastewater treatment plant

Symbols

$\alpha_i$ Correlation coefficients corresponding to the contribution $f_i$
$\rho$ The error associated with Vesilind-based calculations in SPA
$\rho_f$ The error associated with Vesilind-based flux calculations in SPA
The error associated with Vesilind-based limiting solids concentration calculations in SPA

Intercept of the correlation between and the contribution \( f_b \), m²/d

Pseudo-dispersion coefficient, m²/d

Compression coefficient, m²/d

Pseudo-dispersion coefficient, m²/d

Factor or interactions between factors correlated to \( D \)

Settling tank’s average depth, m

Inlet height in the settling tank, m

Solids flux, kg/m²/s

Limiting solids flux in SPA, kg/m²/s

Operating flux, kg/m²/s

Solids settling flux in SPA, kg/m²/s

Inlet flowrate, m³/d

Overflow rate, m³/d

Underflow rate, m³/d

Recycle ratio, dimensionless

Coefficient of determination, dimensionless

SBH calculated with the 1D model, m

time, h

Bulk velocity, m/s

Sludge settling velocity, m/s

Sludge concentration, kg/m³

Effluent sludge concentration, kg/m³

Inlet concentration, kg/m³

Limiting sludge concentration in the SPA, kg/m³

Underflow sludge concentration, kg/m³

Transient-compression sludge concentration threshold, kg/m³

Vertical direction variable, m

### INTRODUCTION

Effective design, operation and control of secondary settling tanks (SSTs) in activated sludge processes are crucial ways of mitigating climate-induced hydraulic effects and filamentous bulking conditions in wastewater treatment plants (WWTPs) (Ramin et al. 2014a). Extreme hydraulic shock events are expected to occur more often in the future due to climate change (Larsen et al. 2009), and future adaptation and mitigation measures will require models capable of describing WWTP systems performance under the changing flow conditions (Plösz et al. 2003; Jeppsson et al. 2013; Langeveld et al. 2015). SST design is still too often based on heuristic/rule-of-thumb principles (Parker et al. 2001). Furthermore, SST loading capacity determines the maximum permissible load that can enter a WWTP; however, the heuristic nature of SST operation in terms of setting the permissible WWTP influent is still a common approach (Plösz et al. 2009).

Solids-flux theory (SFT) and state-point analysis (SPA) provide a steady-state 1D tool for practitioners concerned with SST design, capacity analysis, and optimising daily operations (Li & Stenstrom 2014a; Gao & Stenstrom 2019). SPA is a practical method for assessing the solids flux transported via SSTs, thereby determining under-, critically or overloaded conditions via the solids handling criteria I and II (Keinath 1983). Design and operation charts were developed (Daigger & Roper 1985) to provide visual representations of the association between the hindered settling velocity and the total suspended solids (TSS) concentration. The stationary behaviour of the conceptual ingredients of the SFT was described by Diehl (2008). The 1D advection-dispersion model is described as a second-order partial differential equation (PDE) model (Bürger et al. 2011) and is represented by the governing conservation of mass equation:

\[
\frac{\partial X}{\partial t} + \frac{\partial (v_B \cdot X)}{\partial z} + \frac{\partial (v_H \cdot X)}{\partial z} = - \frac{\partial}{\partial z} \left( D_{\text{Comp}}(X) + D_{\text{Disp}}(z) \frac{\partial X}{\partial z} \right) + v_{\text{in}} X_{\text{in}}(t) \cdot \delta(z). \tag{1} \]

In Equation (1), \( X \) is the solids concentration, \( z \) is the vertical direction variable, \( v_B \) is the bulk velocity, \( v_H \) is the hindered sludge settling velocity, \( v_{\text{in}} \) is the inlet flow velocity and \( \delta \) is the Dirac delta. \( D_{\text{Comp}} \) and \( D_{\text{Disp}} \) denote compression settling and pseudo-dispersion, respectively. In interpreted computational fluid dynamics (iCFD) (Guyonvarch et al. 2015), the constitutive function for \( D_{\text{Disp}} \) is expressed as a statistical meta-model inference that implicitly accounts for the hydraulic effects by flow and design boundary conditions – i.e. inlet concentration \( (X_{\text{in}}) \), the overflow rate \( (Q_{\text{ov}}) \), recycle ratio \( (R) \), side water depth \( (\text{SWD}) \) and inlet height \( (H_{\text{in}}) \). A focal area chosen for the present study is to quantify the error introduced by SFT by calculating the limiting flux based on the solids-flux theory using the iCFD.

SPA is widely used for predesign to establish clarifier area and return pump capacity (Henze et al. 2008). Additionally, many design standards (e.g., UK-WRC; Germany-ATV; the Netherlands-STOWA) are based on SPA, in which empirical relations are used to account for the intrinsic variabilities and uncertainties. SPA can also be used in operation to assess the maximum mixed liquor suspended solids (MLSS) and \( Q_{\text{RAS}} \) settings (Henze et al. 2008). As
for process control, $Q_{\text{RAS}}$ can be set to a constant value or proportional to the influent flow rate. Diehl (2001) presented control strategies using operating charts to control $Q_{\text{RAS}}$ as a function of the feed concentration, feed mass flux and time. SPA combined with on-line real-time control was proposed (Lynggaard-Jensen & Lading 2006) to limit the sludge blanket height (SBH) in SSTs. The limitations of conventional SPA are that it only considers (i) the vertical dimension and (ii) the hindered settling velocity of activated sludge (Vesilind 1968). Consequently, the impacts on it of horizontal hydraulic motion and the effect of SST design boundaries (notably baffles) are neglected, even if they have been shown to have a crucial effect on the solids distribution in SSTs especially due to turbulence and density currents (Zhou & McCorquodale 1992; Krebs 1995; Parker et al. 2001; De Clercq 2003; Plósz et al. 2007). Additionally, transient and compression settling have been shown to have a significant impact on settling velocity at high solids concentration, and thus on calculating the critical solids flux (De Clercq et al. 2008; Bürger et al. 2011; Ramin et al. 2014b; Guyonvarch et al. 2015; Torfs et al. 2015). The question arises as to how these factors can affect the results obtained in SPA, and how to amend for them in a practical way – the focal area chosen for this study.

For SST design and trouble-shooting, CFD is a powerful tool (Ekama et al. 1997; De Clercq 2003; Water Environment Federation 2005; Karpinska & Bridgeman 2016), but due to its complexity and comparably high computational demand, its use is predominantly limited to single unit process operations. Consequently, the optimisation of mesh resolution as a function of solution accuracy is a major challenge to overcome – a focal area addressed in depth here in the context of SST simulations. To overcome these limitations, 1D modelling tools can be improved using 2D or 3D CFD models (De Clercq 2003; Ekama & Marais 2004; Plósz et al. 2007; Guyonvarch et al. 2015). To provide a consistent 1D modelling tool for systems analysis – e.g., to design and optimise SSTs connected to activated sludge reactor systems – the iCFD modelling framework (Ramin et al. 2014b; Guyonvarch et al. 2015) has been developed. In iCFD, statistical meta-models are inferred and used to calculate $D_{\text{Disp}}$ by considering a broad range of design and flow boundary conditions, capturing multi-dimensional phenomena via the calibration of $D$ using 2D CFD simulation outputs. We note that, for practitioners, iCFD can offer a simple, implicit representation of design and flow-boundary conditions using the embedded statistical meta-models. Whilst developed using complex multi-dimensional CFD simulations, 1D iCFD can potentially allow practitioners to make predictions on complex hydrodynamics and transport phenomena without the burden of having to use highly complex simulation tools.

Finally, Belia et al. (2009) propose avoiding the use of semi-arbitrary SF, and, instead, derive SF from quantifications of the uncertainty in simulation models, thereby providing stakeholders with the ability to explicitly include risk evaluations in their decision making process.

The main objective of this study was to quantify and amend the results obtained using the solids-flux theory by assessing the significance of impacts propagating from boundary conditions and settling behaviour on the limiting flux calculations. Therefore, the set of aims defined comprised: (i) reducing uncertainties propagating from CFD by optimising the mesh generation for SST CFD simulations; (ii) assessing the impacts of hindered-transient-compression settling velocity as well as of selected design and flow boundary conditions on the limiting flux and limiting concentration using a 1D iCFD simulation model; (iii) assessing the sensitivity of SHC I, (Ekama et al. 1997) limiting conditions to the individual and combined effects of the selected boundary conditions; (iv) proposing a practical approach to amend for the intrinsic uncertainties of SHC I in SPA.

**MATERIAL AND METHODS**

**CFD simulations**

The CFD simulations were carried out using the open source software package OpenFOAM® (OpenFOAM Foundation). The iterative settlingFoam solver by Brennan (2001) extended by Ramin et al. (2014b) was used to determine the hydrodynamic behaviour and solids distribution inside the SST. The solver was modified to account for hindered, transient and compression settling regime, and the Herschel–Bulkley sub-model was implemented and calibrated to simulate sludge rheology.

**Mesh generation**

To decrease the uncertainties (numerical dispersion) propagating from the CFD to the iCFD structure – and thus to our observations on SPA – a study on optimising the mesh used for SST CFD simulations was carried out based on a comprehensive literature review (Table 1).

The base mesh case was that presented by Ramin et al. (2014b). A wide range of design and flow boundary conditions – in terms of SST design features and sizing – were
The iCFD 1D advection dispersion model for SST simulation model

The iCFD 1D advection dispersion model for SST (Guyonvarch et al. 2015) – developed using the 2D axi-symmetrical CFD model – was employed to compute the local solids concentration and limiting flux curves. The iCFD tool is based on a 1D second-order advection dispersion model. Its main features are: (i) the SST surface area is assumed to be constant and equal to the tank surface area; (ii) to keep the same volume between CFD and 1D model, the 1D depth is taken equal to the average surface area; (ii) to keep the same volume between CFD and 1D model, the 1D depth is taken equal to the average surface area; (iii) a moving feed layer is used in order to take into account the buoyancy effect of the density current according to Dupon & Dahl (1995) and Guyonvarch et al. (2015). In brief, the feed layer is located in the highest layer having a concentration greater than \( X_m \) in the tank; (iv) for each time-step, \( D_{Disp} \) is calculated as a function of design and flow boundary conditions and it has the same value along the tank; (v) the settling velocity model by Ramin et al. (2014b) and Guyonvarch et al. (2015) is implemented, including hindered settling (Takács et al. 1991):

\[
\nu_{H} = v_0(e^{-r_{r}X} - e^{-r_{r}X})
\]

where \( v_0 \) is the maximum settling velocity; \( r_H \) and \( r_P \) are the hindered and low concentration indices, respectively. Additionally, it accounts for transient and compression settling velocity (\( D_{Comp} \)) defined as

\[
D_{Comp} = v_0 e^{-r_{r}X} \cdot \frac{\rho_s}{\rho_s - \rho_l} \cdot g \cdot \frac{(X - X_{TC})}{C_1} \cdot C_2
\]

where \( v_{0,t} \) and \( r_t \) are the maximum transient settling velocity and concentration index, respectively; \( \rho_s \) and \( \rho_l \) are the sludge and water density, respectively; \( g \) denotes the gravity constant; \( C_1 \) and \( C_2 \) are parameters in the effective solids stress derivative (\( \partial\sigma/\partial X \)). The complete solids settling function is given as:

\[
v_s = \left\{ \begin{array}{ll}
v_{H} & \text{if } X \leq X_{TSS,C} \\
D_{Comp} & \text{if } X > X_{TSS,C}
\end{array} \right.
\]

Importantly, this settling model has been validated against full-scale measurements using a 2D axi-symmetrical CFD model implementation (Ramin et al. 2014b); (vi) for model calibration, \( X_{TC} \) is set according to Ramin et al. 2014b and Guyonvarch et al. (2015), i.e. it is equal to the sludge concentration of the first layer below the feed layer; (vii) for the 1D model discretisation, 200 layers are used.

### Table 1 | Optimisation of the mesh characteristics

<table>
<thead>
<tr>
<th>Mesh feature</th>
<th>Value/Specifics</th>
<th>Comments</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mesh type</td>
<td>Polyhedral</td>
<td>Found to be the best adapted based on literature</td>
<td>Ferziger &amp; Peric (1996); Ramin et al. (2014b)</td>
</tr>
<tr>
<td>Local refinement</td>
<td></td>
<td>• Localisation: Inlet, effluent outlet and sludge outlet (inlet + outlets)</td>
<td>Ferziger &amp; Peric (1996)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Minimum size (relative to base size): 15%</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Target size (relative to base size): 30%</td>
<td></td>
</tr>
<tr>
<td>Surface growth rate</td>
<td>1.1</td>
<td>• Surface growth rate defines the maximum size ratio between two neighbouring faces</td>
<td>Ferziger &amp; Peric (1996)</td>
</tr>
<tr>
<td>Base size</td>
<td>0.1 m</td>
<td>Even a coarse mesh, of around 6,000 cells, has been proven to give accurate results for the base case</td>
<td>Ramin et al. (2014b)</td>
</tr>
<tr>
<td>Number of cells</td>
<td>6,176</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
We note that, even if 60 layers have been shown to be an effective trade-off between computational time and minimisation of the numerical error, 200 layers were used here to observe sufficient number of points in the compression zone, even at low SBH. The 1D iCFD simulation model used to test SFT was developed using 50 different (Latin hypercube sampling, LHS) design and flow boundary sets, as well as 36 independent sets for factor screening, thus totalling 86 different 2D axi-symmetric circular conical SST tank designs and operational conditions. Using the average 1D profiles generated using the CFD simulation results, the 1D model development included the rigorous testing of four different dispersion models and different assumptions of critical solids concentration for the onset of compression settling, amongst others (Guyonvarch et al. 2015). The resulting statistical meta-model inferred between \( D_{\text{Disp}} \) and the five most significant flow and design boundary conditions by (Guyonvarch et al. 2015) is as follows:

\[
D_{\text{Disp}} = \left[ -19.96 + 5.64 \cdot X_{\text{In}} + 9.014 \cdot R - 1.76 \cdot H_{\text{Int}} + 241.5 \cdot Q_{\text{SWD}} - 0.66 \cdot X_{\text{In}}^2 + 0.911 \cdot X_{\text{In}} \cdot H_{\text{Int}} - 2.4 \cdot R \cdot H_{\text{Int}} - 53.7 \cdot X_{\text{In}} \cdot Q_{\text{SWD}} + 0.268 \cdot \text{SWD} \right]
\]  

This meta-model multi-dimensional phenomena to be captured implicitly – factors that cannot be explicitly described in a 1D model structure, e.g., turbulence, density currents, and design boundary conditions.

**1D settling flux modelling**

For each of the 200 layers, the local solids concentration \( X \) and the local settling flux \( J_s \) were computed using the iCFD model implemented in MATLAB® (MathWorks Inc.) according to \( j_s = v_S(X) \cdot X \). For each of the 50 experiments, the iCFD model was run with the corresponding calibrated \( D \). Finally, the settling flux curves were plotted. Based on the obtained settling flux curve, the total solids flux \( J \) can be obtained as a function of \( X \), according to:

\[
J = J_S + \frac{Q_{\text{RAS}} \cdot X}{A}
\]  

\( J_L \) and the associated \( X_L \) were determined for each of the 50 experiments using MATLAB® (Table S1, Supporting Material).

**Statistical calculations**

To identify factors and multi-factor interactions that can significantly impact \( J_L \) and \( X_L \), statistical analysis was performed using the JMP® software (SAS Institute Inc.). Through linear regression, meta-models \( (b_i + \sum \alpha_i \cdot f_i) \) were developed for \( X_L \) and \( J_L \), as well as for the discrepancies between \( \rho_I \) and \( \rho_X \) obtained using the conventional SPA and the iCFD-based approach. The meta-model parameters are provided in terms of intercept \( (b_i) \) and coefficient \( (\alpha_i) \) associated to each contribution of factors \( (f_i) \). As for model validation, the accuracy of the meta-models is assessed using 1D iCFD simulation model predictions.

**MESH OPTIMISATION**

The results obtained with the optimised mesh – the best trade-off obtained between accuracy and computational time to reach steady state (Figure 1) – closely agree with those obtained with the base case mesh by Ramin et al. (2014b) that were validated using full-scale measurements.

**Figure 1** | Schematic view of the 2D axi-symmetrical mesh developed with enlarged image demonstrating the inlet mesh refinement. The mesh is a coarse mesh (cell base size: 0.1 m), locally refined around the inlet and the outlets (relative minimum size: 15%, relative target size: 30%, surface growth rate: 1.1). Please refer to the online version of this paper to see this figure in colour: http://dx.doi.org/10.2166/wst.2020.090.
(Figure S1, Supporting Material). Additionally, a gain in convergence and stability of the numerical solution was achieved using the optimised mesh scheme (Figure S2).

To assess the optimal mesh size, a finer mesh (around 15,000 cells) and a coarser one (around 3,000 cells) were compared to the coarse mesh (around 6,000 cells). Mesh characteristics used are presented in Table S2. The boundary conditions employed were those by Ramin et al. (2014b). Results obtained, in terms of TSS concentration and radial velocity profiles (Figure 2), suggest that the finer the mesh, the more slowly convergence is reached. Therefore, using the coarser mesh can be used to allow saving CPU time.
However, as shown in Figure 2, a gradual deterioration of the numerical solution – in terms of average radial velocity and TSS concentration profile – is observed when decreasing the number of cells from 6,000 to 3,000. Therefore, a coarse mesh was selected for further assessment as it can allow an effective trade-off between the accuracy of the solution and computational time.

Moreover, while keeping the number of cells ~6,000, the mesh was further optimised by changing local refinements and surface growth rate. The mesh characteristics used for the optimisation – in terms of local refinements, surface growth rate and number of cells – is presented in Table S3. The obtained radial velocity and TSS concentration profiles averaged along the tank (Figure 3) indicate that: (i) applying a refinement to the bottom slope seems to worsen the solution; (ii) mesh generated with higher surface growth rate (Coarse 2) and with lower inlet and outlets refinements (Coarse 3) result in very similar simulation outputs; (iii) the real execution time needed to reach steady state is similar in all three cases (i.e. Coarse, Coarse 3 and Coarse 4), and no significant gains could be obtained by increasing surface growth rate (Coarse 3) or by decreasing local refinements (Coarse 4).

Finally, the mesh quality was assessed using a critically loaded case, where the sludge blanket reached the inlet baffle as shown in Table S4 (Exp #16 of the first factors screening study in Guyonvarch et al. 2015). Importantly, no local refinements were considered around the baffles, at the interface between the clear zone and the sludge blanket, even if high velocity variations were observed at this location. The target output values obtained are similar for both meshes (less than 10% relative error), except for the peak radial velocity (21% relative error). However, the long term objective being 1D model development, only the TSS distribution was considered. Therefore, these results support the choice of the presented coarse mesh (Figure 1), with only inlet and outlet local refinement, as a benchmark for mesh construction.

**RESULTS AND DISCUSSION**

**Quantify uncertainties intrinsic to conventional SPA**

The solids distribution in the tank was determined for the 50 LHS experiments (Table S5, Supporting Material).

Additionally, the settling flux was computed for each layer for the 50 LHS experiments – obtained using hindered (Vesilind) and hindered-transient-compression (Ramin) velocity terms is shown in Figure 4. The settling flux curves follow the Vesilind-based curve until \( X_{TC} \), then the settling flux is significantly lowered, thus indicating a significant degree of correction necessary to calculate SHC 1. We note that, in the simulation model, values of \( X_{TC} \) were set equal to the concentration of the first layer below the feed layer (denoted as \( X_{In} \)). For each of the 50 LHS experiments \( J_L \) and the associated \( X_L \) were determined based on the total solids-flux curves (Figure 5; Table S1).

**Figure 4** | Settling flux [kg/m²/s] as a function of local solids concentration [g/L] for the 50 experiments design using LHS including transient and compression settling in the model (Ramin settling) (dots) (Guyonvarch et al. 2015). The colour of the dots corresponds to initial concentration \( X_{In} \) [g/L] of the corresponding experiments. The solids line represents the settling flux curve when only hindered settling is considered (Vesilind settling). Please refer to the online version of this paper to see this figure in colour: http://dx.doi.org/10.2166/wst.2020.090.

**Figure 5** | Total solids flux [kg/m²/s] as a function of the local solids concentration [g/L] for the 50 experiments design using LHS including transient and compression settling in the model (Ramin setting) (dots) (Guyonvarch et al. 2015). The colour of the dots corresponds to initial concentration \( X_{In} \) [g/L] in the corresponding experiments. Please refer to the online version of this paper to see this figure in colour: http://dx.doi.org/10.2166/wst.2020.090.
The error ($\rho$) obtained using the Vesilind-based fluxes was quantified by determining the limiting flux and concentration values for the 50 LHS experiments (Figure 5; Table S6). A statistical analysis (Table 2) of $J_L$ and associated $X_L$ as well as of $\rho_L$ and $\rho_X$ indicated strong dependency on the loading conditions and on $R$. Design boundary factors ($H_{in}$ and SWD) were found not to significantly impact the calculation of the total solids-flux curve. $X_L$ and $J_L$ were correlated with the loading conditions through Equations (7) and (8) with $R^2 = 0.998$ and 0.996, respectively (and adjusted $R^2 = 0.998$ and 0.996, respectively).

$$X_L = -4.239 + 7.125 \cdot X_{in} - 2.525 \cdot R + 20.986$$

$$J_L = 0.00148 + 0.000683 \cdot R - 0.00989 \cdot Q_{ow} - 0.000659$$

$$X_{in} = 10.821 \cdot Q_{ow} + 0.000985 \cdot R^2 + 0.00723 \cdot Q_{ow} \cdot R + 0.0045$$

$$X_{in} = 16.305 \cdot Q_{ow} + 0.000834 \cdot Q_{ow} \cdot Q_{ow} - 0.00041$$

### Table 2

<table>
<thead>
<tr>
<th>Limiting concentration $X_L$ [g/L]</th>
<th>Limiting flux $J_L$ [kg/m²/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R^2 = 0.998$</td>
<td>$R^2 = 0.996$</td>
</tr>
<tr>
<td>Intercept $b_i$</td>
<td>Contribution $f_i$</td>
</tr>
<tr>
<td>$X_{in}$</td>
<td>-38.07° t-ratio -95.43</td>
</tr>
<tr>
<td>$R$</td>
<td>-2.525</td>
</tr>
<tr>
<td>$X_{in} \cdot X_{in}$</td>
<td>-0.606</td>
</tr>
<tr>
<td>$X_{in} \cdot Q_{ow}$</td>
<td>-10.821</td>
</tr>
<tr>
<td>$Q_{ow}$</td>
<td>20.986</td>
</tr>
<tr>
<td>$X_{in} \cdot R$</td>
<td>-2.658</td>
</tr>
<tr>
<td>$R \cdot R$</td>
<td>2.002</td>
</tr>
<tr>
<td>$X_{in} \cdot X_{in} \cdot R$</td>
<td>0.317</td>
</tr>
<tr>
<td>$R \cdot Q_{ow}$</td>
<td>9.499</td>
</tr>
<tr>
<td>Discrepancy $\rho_L$ [-1]</td>
<td>$R^2 = 0.917$</td>
</tr>
<tr>
<td>Intercept $b_i$</td>
<td>Contribution $f_i$</td>
</tr>
<tr>
<td>$X_{in} \cdot Q_{ow}$</td>
<td>11.879</td>
</tr>
<tr>
<td>$X_{in} \cdot X_{in}$</td>
<td>0.0838</td>
</tr>
<tr>
<td>$X_{in}$</td>
<td>-0.874</td>
</tr>
<tr>
<td>$Q_{ow} \cdot X_{in}$</td>
<td>146.286</td>
</tr>
<tr>
<td>$X_{in} \cdot X_{in} \cdot Q_{ow}$</td>
<td>-0.742</td>
</tr>
<tr>
<td>$X_{in} \cdot Q_{ow} \cdot Q_{ow}$</td>
<td>-30.963</td>
</tr>
<tr>
<td>$X_{in} \cdot X_{in} \cdot Q_{ow} \cdot R$</td>
<td>-0.000834</td>
</tr>
<tr>
<td>$Q_{ow}$</td>
<td>-38.100</td>
</tr>
<tr>
<td>$R$</td>
<td>0.0103</td>
</tr>
</tbody>
</table>

Through linear regression, a meta-model is built for each parameter, provided in terms of intercept ($b_i$) and coefficient ($\alpha_i$) associated to each contribution ($f_i$). These coefficients allow the deduction of the correlation expression in the form of $\beta_i + \sum \alpha_i f_i$. The considered factors are $X_{in}$: inlet solids concentration (g/L); $Q_{ow}$: overflow rate (m²/s); $R$: recycle ratio (-); SWD: side water depth (m); $H_{in}$: distance between the top of the tank and the inlet (m).
Quantifying the uncertainty in predicting the limiting flux and concentration

The discrepancies between $\rho_J$ and $\rho_X$ obtained using the conventional SPA – assuming only hindered settling modelled using the Vesilind settling model – and the iCFD-based approach – employing the Ramin settling velocity model (Ramin et al. 2014b; Guyonvarch et al. 2015) – were quantified for the 50 LHS experiments (Table S1). Statistical analysis of $\rho_J$ and $\rho_X$ was performed, and the parameters found to significantly impact these two outputs are shown in Table 2 and Table S6. $\rho_X$ and $\rho_J$ were found to be correlated with the loading conditions through Equations (9) and (10) with $R^2 = 0.917$ and 0.751, respectively, (and adjusted $R^2 = 0.897$ and 0.710, respectively).

$$\rho_X = 1.979 - 0.874 \cdot X_{\text{In}} - 38.1 \cdot Q_{\text{Ov}} + 0.0103 \cdot R$$
$$+ 0.0838 \cdot X_{\text{In}} + 11.879 \cdot X_{\text{In}} \cdot Q_{\text{Ov}} + 146.286$$
$$\cdot Q_{\text{Ov}}^2 - 0.742 \cdot X_{\text{In}}^2 \cdot Q_{\text{Ov}} - 30.963 \cdot X_{\text{In}} \cdot Q_{\text{Ov}}^2$$
$$- 0.000834 \cdot X_{\text{In}}^2 \cdot R$$

(9)

$$\rho_L = -6.994 + 0.653 \cdot X_{\text{In}} + 230.148 \cdot Q_{\text{Ov}} + 0.0475$$
$$\cdot R - 0.0414 \cdot X_{\text{In}}^2 - 2.64 \cdot X_{\text{In}} \cdot Q_{\text{Ov}} - 3291.756$$
$$\cdot Q_{\text{Ov}}^2 + 16303.276 \cdot Q_{\text{Ov}}^3$$

(10)

To validate the statistically identified meta-models, results obtained with Equations (7)–(10) were benchmarked against predictions obtained with the 1D iCFD tool (Figure 6).

Relatively high accuracy of the statistical meta-model was obtained for all four parameters, i.e. $R^2 \geq 0.92$, thereby validating the set of statistical inferences. Additionally, to express the precision and repeatability of the method, the coefficient of variation (CV; the ratio between standard deviation and mean) was calculated (Table S6). For $J_L$, the CV obtained is relatively low, and thus the discrepancies between data obtained using the conventional SPA and the iCFD-based approach could be characterised with an average value of 23% (Figure 7(a); Table S6).

This interpretation of the uncertainty in $J_L$ closely agrees with the reduction SF (25%) reported in earlier computational assessments, excluding compression settling
behaviour (Ekama & Marais 2004) and experimental studies (Ekama & Marais 1986; Ekama et al. 1997; Wilén et al. 2004; Henze et al. 2008). In contrast, for XL, the coefficient of variation is significantly higher (Figure 7(b); Table S6). To interpret the uncertainties in calculating XL using conventional SPA, Equation (9) can be used as it has a comparably high $R^2 = 0.897$. Taken together, a practical approach is proposed to make up for uncertainties pertinent to SHC I in conventional SPA by employing a factor of 23% and using the meta-model Equation (9) to correct JL and XL, respectively.

Using Equations (9) and (10) to amend SFT-based calculations for optimising SST operation would require practitioners benchmarking predicted JL and XL data against onsite measurements and 1D simulation model results.

**Application of the method – an example**

In Guyonvarch et al. (2015), the obtained CFD results for the first factors screening study (see Figure 4 of Guyonvarch et al. 2015) disagreed with the predictions made using conventional SPA (see Figure 3 in Guyonvarch et al. 2015). Briefly, in the screening study, nine load and design parameters were considered in a two-level fractional factorial design of experiments, also comprising different factors related to inlet and effluent baffles. According to conventional SPA, only low sludge blanket was expected for the 16 experiments. However, for experiments #9, #13, #14, #15 and #16, high sludge blanket was predicted by the CFD model accounting for transient and compression settling and validated through real-scale measurements (Ramin et al. 2014b). The correlations obtained between the limiting flux and concentration and the loading condition are very significant ($R^2$ values very close to 1). Therefore, applying the correlation Equations (7) and (8) to the 16 cases of the first factors screening study may help to understand the discrepancy between Vesilind SPA and numerical experiments.

For the 16 experiments, values of JL were predicted using Equation (8) and compared with the operating flux, JOp, calculated according to:

$$J_{Op} = \frac{X_{In} \cdot Q_{In}}{A}$$

(Table 3.) For experiments #9, #10, #12, #13, #15 and #16, JOp ∼ JL was obtained, thereby indicating critically loaded SST conditions. These results are in close agreement with the CFD simulations, showing comparably high sludge blanket, and thus indicating critical loading conditions.

**CONCLUSIONS**

The present study focused on quantifying and amending the results obtained using SFT on secondary settling tanks. The iCFD process modelling framework was used to explicitly account for hindered-transient-compression settling and included implicit statistical inferences (meta-models) for design and flow boundary conditions.
A practical approach is proposed to amend for uncertainties pertaining to SCH I by employing a factor of 23% and using a meta-model to correct values of $J_L$ and $X_L$, respectively, obtained using conventional SPA.

### References


### Table 3

Limiting flux ($L$) predicted using Equation (3) and the actual operating flux applied in the 16 extreme scenario CFD simulations used for the factors screening study in Guyonvarch et al. (2015)

<table>
<thead>
<tr>
<th>Exp #</th>
<th>Limiting flux $L$ $10^{-4}$ kg/m²/s</th>
<th>Operating flux $J_{op}$ $10^{-4}$ kg/m²/s</th>
<th>$L - J_{op}$ $10^{-4}$ kg/m²/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>10.5</td>
<td>3.5</td>
<td>7.0</td>
</tr>
<tr>
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<td>3.5</td>
<td>7.0</td>
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<tr>
<td>3</td>
<td>16.5</td>
<td>5.0</td>
<td>11.5</td>
</tr>
<tr>
<td>4</td>
<td>16.5</td>
<td>5.0</td>
<td>11.5</td>
</tr>
<tr>
<td>5</td>
<td>12.8</td>
<td>7.3</td>
<td>5.5</td>
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<td>26.1</td>
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<tr>
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<td>26.3</td>
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<td>0.3</td>
</tr>
</tbody>
</table>

The corresponding difference between the two fluxes is presented. The negative values are highlighted in orange and the positive values close to zero in yellow. Please refer to the online version of this paper to see this table in colour: http://dx.doi.org/10.2166/wst.2020.090.

### Supplementary Material

The Supplementary Material for this paper is available online at https://dx.doi.org/10.2166/wst.2020.090.


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