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Model identification for hindered-compression settling velocity

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Abstract
Two of the key questions regarding secondary settling are (a) Does a process model exist for which all hindered and compression settling velocity parameters can be estimated using experimental data?; (b) What is the minimum data that need be inferred, from a settling sensor setup to identify process models?” This international research effort aimed to address these questions by carrying out a comprehensive practical identifiability assessment of constitutive functions for hindered and compression settling velocity using laboratory-scale measurements and one-dimensional (1-D) simulation models. For model validation, the triangulation technique was used, including independent laboratory- and full-scale measurements as well as 1-D and computational fluid dynamics (CFD) simulation models.

Keywords
Activated sludge settling velocity; computational fluid dynamics (CFD); model identification.

INTRODUCTION
Parameter identifiability of activated sludge settling velocity models remains a challenge. The increasing frequency of hydraulic shock events – as a result of climate change – necessitates more effective operation and control of secondary settling tanks (SSTs) in wastewater treatment plants (WWTPs) in the future (Ramin et al., 2014a). Theoretically, the maximum permissible SST loading capacity determines the maximum permissible hydraulic WWTP load. However, the SST capacity varies with sludge settleability, and thus process operation and control necessitates effective sensor technology and identifiable simulation models (Jeppsson et al., 2013; Plósz et al., 2009). Settling sensors should ideally provide experimental data for estimating settling velocity parameters; yet, up to date, no simple and robust methods exist to calibrate hindered and compression settling parameters. Derlon et al. (2017) present a cost-effective camera-based method to monitor sludge blanket height (SBH). Ramin et al. (2014b) propose a sensor setup with a TSS sensor installed in the bottom of a settling column, thus inferring SBH and the TSS concentration (X_TSS,bottom) time-series. Valverde-Pérez et al. (2017) demonstrate, however, that SBH and X_TSS,bottom time-series do not provide sufficient information for reliable model identification, and proposed a novel sensor setup, additionally monitoring TSS concentration at different heights in the side of the column (X_TSS,side). Results obtained using state-of-the-art settling velocity models (Torfs et al., 2017; Ramin et al., 2014) still suggest limitations in terms of practical identifiability of compression settling velocity model parameters – in line with work by Li and Stenstrom (2016). As for the uncertainty
sources associated with settling model identification, the design of settling column setups can significantly influence measured data and thus the parameter estimates (Vanrolleghem et al., 1996; Ekama et al., 1997). However, more research is still needed to understand better how the impact of column size propagates to model parameters estimated. Additionally, this study addresses the uncertainty source represented by the use of 1-D simulation models for estimating model parameters, which are subsequently used to calibrate CFD simulation models. Triangulation is the strategic use of multiple inquiries to address the same question, each depending on different set of assumptions with their strengths and weaknesses (Lawlor et al., 2016). Results agreeing across different inquiries are more likely to be replicated reliably.

The aims set in this study are (1) identifying a process model for hindered-compression settling velocity for which all parameters can be estimated using the experimental data with both good settling and filamentous bulking; (2) evaluating the feasibility of the sensor setup as a means to infer experimental data on compressive solid stress; (3) assessing uncertainty sources associated with the model identification method and the settling column design; and (4) evaluating and validating the new settling velocity process model using the triangulation approach.

MATERIALS AND METHODS

Sampling and sensor setup. Activated sludge samples were collected in three WWTPs in Denmark (Fredericia and Avedøre WWTPs) and one in Sweden (Ellinge) with well-settling characteristics (Fredericia and Ellinge with SVI3.5≤90 ml/g) and filamentous bulking (Avedøre, SVI3.5~200 ml/g). The three activated sludge processes differed in terms of operating conditions. Secondary biological treatment in Avedøre WWTP (320 000 PE – mostly municipal sewage) and Fredericia WWTP (350 000 PE – mostly municipal sewage) were operated at solids retention time, SRT=10-15 days, and used polymers and chlorination for bulking control, respectively. Ellinge WWTP (330 000 PE – mostly food industrial wastewater) was operated as a high-rate system, SRT~2 days, without any bulking control measure taken. Settling tests were carried out using the sensor prototype by Valverde-Pérez et al. (2017), which consists of a column equipped with TSS SOLITAX (Hach, USA) infrared sensors installed at 0.21m height in the side wall and in the bottom of the column.

Figure 1. The multi-probe sensor prototype developed equipped with two SOLITAX TSS sensors installed in the bottom and the sidewall of the settling column as well as an image analysis-based sensor with an immersed internal visible light source; (b) TSS values measured at the bottom of the settling column (X\text{TSS,Bottom}) versus experimental time and regression lines used to estimate X\text{TSS,Infi} values for the four settling experiments with Fredericia WWTP sludge;
Image analysis based sensor (camera) and the immersed light source are used for measuring SBH and also to provide parallel TSS\textsubscript{Side} measurements (Fig. 1a). In the full-scale monitoring, a SOLITAX and a SONATAX (Hach, USA) probes were used to measure the SBH and the TSS in the bottom of the SST in the OBVA WWTP, Vila-Real, Spain. For measuring the SBH, the threshold TSS concentration was set to 0.3 kg m\(^{-3}\).

**Identifiability analysis.** The identifiability analysis and model calibration were done using the Latin-Hypercube-Sampled-priors-for-Simplex (LHSS) global method (Wágner et al., 2015). In the LHSS, the Janus coefficient (\(J\)) is used to assess the impact of parameter value variability – for cases with covariance >0.6 – via relative predictive accuracy obtained using the upper and lower parameter boundaries. If \(J\approx1\), then we conclude we have identified parameters. 1-D simulation models were implemented in Matlab (Matworks). The Akaike's information criterion (AIC) was used for model discrimination (Torfs et al. 2017).

**Regression analysis.** Values of the maximum solids concentration \(X_{TSS,\text{Infh}, \text{kg m}^{-3}}\) are estimated using the \(X_{TSS,\text{Bottom}}\) data series obtained for each settling experiment using the regression equation

\[
X_{TSS,\text{Infh}} = \frac{1}{(1-e^{-k_X t})} (X_{TSS,\text{Bottom}}(t) - f_X)
\]

Eq. 1

in SigmaPlot 13 with \(k_X\) and \(f_X\), denoting regression parameters (Fig. 1b).

**CFD simulations.** The software ANSYS-CFX\textsuperscript{®} (Academic Res. Release 17.2) was used to develop the solver according to Ramin et al. (2014b). That is the solver employs an average Eulerian 2-phase flow model. Turbulence is modelled using the \(k-\varepsilon\) model. Molecular viscosity of sludge is predicted using the Herschel-Bulkley model. Additionally, the solver included the novel hindered-compression settling model implementation. The initialization of the 2-day transient state was explored by three different approaches: (1) defining intuitively a SBH with a constant TSS; (2) converging a previous steady-state case with a constant influential flow; (3) using a transient state (very costly in terms of computing time). The second choice of initialisation was eventually used. For simulating the column, the wall-with-no slip and smooth roughness were used with fluid velocity on the walls equalling zero.

**Model validation by triangulation (MVT).** The MVT addresses the question of reliable prediction of hindered and compression settling using the process model developed. MVT comprises two independent approaches, i.e. (a) practical model identification using two independent sets of laboratory-scale measurements (Ellinge and Avedøe) using the 1-D simulation model; and (b) forward simulations of independent sets of dynamic full-scale measurement data (SBH and \(TSS_{\text{RAS}}\)) using a CFD solver developed. Key sources of bias for approaches \(a\) and \(b\) are the highly degenerated simulation model structure in 1-D and the lack of estimation of parameter values other than settling velocity parameters through the calibration of the CFD simulation model, respectively. No specific direction of bias of these sources can be made explicit. Results from these two approaches are compared through the CFD simulation of column tests for well-settling and filamentous sludge (Fig. 6).

**Assessment of two uncertainty sources.** One of the sources of uncertainty assessed using CFD simulations, involved the design boundary conditions of the settling column setup. The impact of the column sensor design on the model parameters estimated was tested via forward CFD simulations, whereby the CFD solver was calibrated with model parameters obtained for the Fredericia sludge at 3.44 g l\(^{-1}\) as initial concentration (Fig. 2) and the Avedøe sludge at 3.86 g l\(^{-1}\) as initial concentration (Fig. 4). The base case scenario (\(F=1\)) was that of the real setup (Fig. 1a), and
factors (e.g., F=0.7 means 70%) were applied to resize the height and diameter of the column, maintaining the original proportions. Additionally, the approach of using 1-D simulation models for estimating parameters – that are then used to calibrate CFD simulation models – was identified and assessed as an additional uncertainty source. The predictive efficiencies of the 1-D and the 2-D CFD simulation models were benchmarked using measured data obtained with the Fredericia sludge at X\text{ini}=3.44 g/l as initial concentration.

RESULTS AND DISCUSSIONS

Model identification. Through an iterative approach, involving testing the practical identifiability of parameters in a plethora of rate equations, including 2-parameter (2P) modified power, 3P sigmoidal and 3P exponential, a 3P exponential term was identified to describe compressive solids stress gradient, i.e.

\[ v_g = \begin{cases} 
\nu_H \nu_{0e^{-\rho S X_{TSS,I}}}, & X_{TSS,I} \leq X_{TSS,C} \\
\nu_H \left(1 - \frac{\rho_S}{\rho_S - \rho_f} g z X_{TSS,I} \right), & X_{TSS,I} > X_{TSS,C}
\end{cases} \]

where the effective solids stress (\( \tau \)) gradient is formulated with \( \nu_C \) (m\(^2\) s\(^{-2}\)) and \( \nu_C \) (-) parameters. The maximum solids concentration (\( X_{TSS,I} \), kg m\(^{-3}\)) is used to normalise local biomass concentration values \( X_{TSS,I} \). For hindered settling velocity (\( v_H \), m s\(^{-1}\), the model includes a pseudo 2-parameter exponential constitutive function with \( v_0 \) (m s\(^{-1}\)) and \( r_H \) (m\(^3\) kg\(^{-1}\)), denoting the hindered settling velocity parameters. For hindered settling, the 3-parameter logistic function by Diehl (Diehl, 2015; Torfs et al., 2017) was also tested, in combination with the new compression model with parameters shown in (Fig. 2).

![Figure 2](image.png)

**Figure 2.** Measured and simulated data for solids collected in Fredericia WWTP, posterior parameter probability distributions, covariance matrix; AIC assessed using the new hindered-compression process model and the Diehl hindered settling model combined with the new compression model.

Furthermore, in Eq. 2, \( \rho_S \) and \( \rho_f \) are the sludge and water density, respectively; \( g \) denotes the gravity acceleration constant; \( z \) is the depth in the settling column. For simulating batch settling tests and SST, the compressive threshold concentration (\( X_{TSS,C} \)) is set to the initial solids concentration and the influent TSS, respectively (Guyonvarch et al., 2015). Instead of letting
parameters independently vary, the ratio of $v_0/r_H$ was identified with $v_0$ set as constant (0.0025, m d$^{-1}$). The $v_0/r_H$ ratio gives a good indication of settling properties and can be linked, notably, to the degree of sludge bulking (Wagner et al., 2015) which makes it a good controlled parameter. The novel process model requires only three parameters to estimate ($v_0/r_H$, $v_C$, $r_C$) – all practically identifiable using the experimental data obtained using the sensor. That is posterior parameter distributions (Fig. 2) show comparably narrow confidence intervals, and although, the covariance matrices show values $>0.6$ for compression parameters in some cases, parameter variability does not significantly influence simulation outputs, i.e. $J$~1. (data not shown).

**Validation using independent batch settling data.** Independent experimental settling data – obtained using solids with well-settling and filamentous bulking characteristics – were used to test practical identifiability of and to validate the simulation model structure (Fig. 3 and Fig. 4).

![Table 1](image)

**Figure 3.** Measured and simulated data for solids collected in Ellinge WWTP, posterior parameter probability distributions (obtained using 250 LHSS simulations), covariance matrix.

As for the Ellinge data (Fig. 3), results obtained show close agreement with the outcomes in the Fredericia case (Fig. 2) in terms of predictive accuracy and parameter covariance. TSS$_{side}$ is effectively predicted through all three experiments. Additionally, at TSS=3.76 g/l, prediction of the SBH improves, which is not the case for the TSS$_{bottom}$ data series, thereby leading to ~1.5 g/l overestimation of the measured data.

![Table 2](image)

**Figure 4.** Measured and simulated data for solids collected in Avedøre WWTP, posterior parameter probability distributions (obtained using 250 LHSS simulations), covariance matrix.

In contrast to the Fredericia and Ellinge datasets, validation using solids collected in Avedøre WWTP extended the model identifiability boundaries to filamentous bulking conditions (Fig. 4).
Again, the outcomes of the identifiability test closely agree with the Fredericia case. Compared to Fredericia and Ellinge cases, improved prediction of the SBH and TSS\textsubscript{bottom} is obtained with bulking sludge. Taken together, the independent results obtained with Ellinge and Avedøre solids suggest the validity of the identifiability approach and the simulation model structure. The reliability of the process model is further supported by the improved predictive efficiency – in terms of both SBH and TSS\textsubscript{Bottom} - under filamentous bulking conditions – an important aspect for future development of model-based control design structures for WWTPs.

**Parameter intervals for the new model.** Fig. 5 summarises all parameter values with confidence intervals obtained with the three solids. As for Fig. 5a., fixing \( v_0 \) was found to allow the estimation of \( v_0/r_H \) values in a narrow range for the different initial concentrations and independently from the compression parameters according to the covariance matrices obtained. This was otherwise impossible to achieve with any of the functions tested. Fig. 5a also supports the hypothesis of \( v_0/r_H \) effectively gauging sludge settling properties (Wágner et al., 2015) with \( v_0/r_H \sim 0.005 \), indicating the boundary between well-settling and filamentous bulking solids.

\[
\begin{array}{c|c|c|c|c}
\text{XIni} & 2 & 3 & 4 & 5 \\
\hline
\text{v}_0/\text{r}_H & 0.002 & 0.004 & 0.006 & 0.008 \\
\text{v}_0 & 0.0 & 0.1 & 0.2 & 0.3 & 0.4 \\
\text{r}_C & 0 & 1 & 2 & 3 & 4 & 5 \\
\end{array}
\]

**Figure 5.** Posterior mean parameter values with confidence interval denoted with error bars for the three WWTPs.

For \( v_C \) – denoting the maximum compressive solid stress gradient parameter – significant dependence on initial solids concentrations is obtained – an observation that cannot be fully supported for \( r_C \) (Fig. 5b and 5c). Notably, \( v_C \) parameter values indicate different trends under well- and filamentous-settling conditions. Under bulking conditions, \( v_C \) values show an approximately ten-fold increase towards low solids concentrations compared well-settling sludge. For the latter case, the trend in \( v_C \) values can be characterised with a minimum range at comparably low initial TSS concentrations – close agreement between Fredericia and Ellinge data – and with a progressive increase towards high initial TSS concentrations. Despite the considerable difference between the three WWTPs in terms of operating conditions - in terms of SRT and bulking control measures – settling parameters obtained show consistent and comparable trends.

**Assessing sources of uncertainty using CFD simulations.** CFD simulations of the settling column setup (Fig. 6; at design factor F=1) indicate negligible uncertainties introduced by the 1-D parameter estimation approach, and thus suggest the reliability of the parameter estimation approach. We note that the improved predictive efficiency of CFD simulation model compared to the 1-D case (Fig. 6a and 6b) – in terms of SBH – suggest that the overestimation of the compressive SBH tail by the 1-D simulation model may be a bias caused by the degenerated 1-D simulation model structure rather than the settling velocity process model structure. The latter was the same in both the 1-D and the 3-D CFD model. Torfs et al., (2017) assessed the effect of overestimation of the compressive SBH tail in more depth, suggesting that the 1-D simulation...
model structure - in terms of hindered settling velocity formulation – as the potential cause of such bias.

**Figure 6.** CFD simulation results obtained using solver calibrated according to parameter values obtained with Fredericia sludge at $X_{\text{ini}}=3.44$ g/l (Fig. 2) at different design similarity factors (F) compared to the real setup (F=1; Fig. 1a). Fig. 6b shows an excerpt of 1-D results from Fig. 2.

Furthermore, to assess the variability of parameter values as a result of settling column design, CFD simulations, carried out within a wide range of column design boundary conditions (Fig. 6), were used to re-estimate settling velocity model parameters (Fig. 7). Results obtained suggest that, with negligible wall effects, only values of $r_C$ can be expected to vary significantly in the wide design boundary range studied for both well- and filamentous sludge settling.

**Figure 7.** Settling model parameters estimated with different column design using CFD simulation output data obtained using calibration parameter sets for well-settling sludge from Fredericia WWTP (a) and sludge with filamentous bulking collected in Avedøre WWTP (b)

*Full-scale measurements and CFD simulations.* As part of the MVT approach, forward CFD simulation results (Fig. 8) closely agree with full-scale SST measurement data collected during more than 40 hours – in terms of SBH and $X_{\text{TSS,RAS}}$. 
Figure 8. Measured and simulated (a) SBH and (b) TSS$_{RAS}$ data for the full-scale SST monitored.

Taken together, both approaches involved in the MVT support the hypothesis that the novel constitutive function for hindered and compression settling velocity can reliably predict the real physical phenomena, thereby validating the process model developed.

Quantifying compressive solid stress using sensor. This study also addressed the question whether the multi-probe sensor setup could be used to quantify the $\tau$-gradient – a variable approximated using the sensor data according to

$$\frac{\partial \tau}{\partial X_{TSS,i}} = \frac{(\rho_s - \rho_L) \cdot g}{(X_{TSS, bottom} - X_{TSS, side}) / h_{side sensor}},$$

Eq. 3

where the density difference between water and sludge ($\rho_s - \rho_L$) was assumed constant. Eq. 3 was identified based on force balance analysis – assuming only the gravitational, buoyancy and solids pressure acting on particles – and by assuming quasi steady-state conditions (Xu et al., 2017). Simulation results obtained (Fig. 9) reasonably agree with the sensor $\tau$-gradient values for sludge with well-settling and filamentous bulking characteristics.

Figure 3. Measured/simulated compressive solid stress using (a) well-settling sludge from Fredericia WWTP and (b) sludge with filamentous bulking collected in Avedøre WWTP.

This result indicates the feasibility of the sensor approach to quantify solid stress. More research is needed to assess the error introduced by assuming quasi steady-state in approximating compressive
solids stress using the sensor data. Additionally, the benefits of using $\tau$-gradient sensor data for settling model calibration will be evaluated.

**CONCLUSIONS**

The concluding remarks drawn in the study include

- A pseudo 2P and a 3P exponential term were identified to describe hindered settling velocity and the compressive solids stress gradient, respectively;
- The ratio of $v_0/r_H$ was estimated with $v_0$ set as constant;
- Three parameters are required to estimate using LHSS ($v_0/r_H$, $v_C$, $r_C$) – all practically identifiable using the data obtained using the innovative multi-probe sensor setup;
- Only $v_C$ shows significant dependence on initial solids concentration;
- The process model developed was validated using the triangulation approach, including independent laboratory- and full-scale measurement data and using 1-D and CFD simulation models;
- Negligible uncertainties – assessed by means of CFD simulations – introduced by the 1-D parameter estimation approach were obtained, thus suggesting the reliability of the practical identifiability assessment approach.
- The multi-probe settling sensor setup developed can be used to quantify the $\tau$-gradient, and future research should assess the benefits of using $\tau$-gradient sensor data for settling model calibration.

**REFERENCES**


