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Practical identifiability and uncertainty analysis of the one-dimensional hindered-compression continuous settling model

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ABSTRACT

The practical application of the one-dimension hindered-compression settling models remains a challenge, since the model calibration strongly depends on experimental observations with limited information. In this study, the identifiability of parameter subsets of the hindered-compression models is evaluated for various experimental layouts. Global sensitivity analysis is used to preliminarily select the influential parameters which can be reasonably estimated, while the identifiability analysis of parameter subsets is conducted based on the local sensitivity functions and collinearity measures. The batch settling curve observations are informative for calibrating hindered parameters, and to determine the compression parameters, the concentration profile observations may need to be collected. For different experimental layouts, at least three parameters are identifiable, and the number of identifiable parameters can potentially increase to five, if both batch settling curve and concentration observations are available. The parameter subset identifiability is sensitive to the choice of initial parameter values, and determining the initial values of hindered parameters and gel concentration by measuring the hindered settling velocities and the top concentration of the static sediment respectively allows efficient reduction of the sensitivity. Parameter subset estimates are sensitive to the values of fixed parameters, and reliable estimation of identifiable parameter subsets is possible to significantly decrease model prediction uncertainties.

1. Introduction

As the mostly used solids-liquid separation unit in wastewater treatment process, secondary settling tanks (SSTs) are able to remove finely dispersed solids to produce low turbidity effluent, and to concentrate the solids in an underflow for it to be recycled or disposed in the least volume. The two functions are known as clarification and thickening. The traditional SST design and operation strategies tend to be empirical and conservative, which may cause an unanticipated performance fluctuation of the SST itself and a low efficiency of energy and land use (Li and Stenstrom, 2014a,b).

For design and operation optimization purposes, various SST mathematical models have been developed to provide a reasonable prediction of the effluent solids concentration, underflow solids concentration, sludge blanket level and sludge inventory which are specifically important during hydraulic shock loading and sludge settleability deterioration. In most commercial simulators, one-dimensional (1-D) SST models are most often used due to their simplicity and less computation burden, especially if long term simulations are needed (Bürger et al., 2011). Most early 1-D models, such as the well-known Takács model (Takács et al., 1991), are derived considering only local mass conservation and hindered settling. In last decade, the improved understanding of activated sludge rheology has facilitated the development of phenomenological theory of sedimentation-consolidation, which provides a more rigorous description of the compression settling behavior (Bürger, 2000). The phenomenological theory is subsequently expressed in the 1-D model from the mass and linear momentum balance, allowing the development of hindered-compression models, such as the Bürger-Diehl model (Bürger et al., 2012, 2013). Compared with the hindered-only models, the hindered-compression models have the advantage of providing improved compression settling simulations, thus allowing more accurate predictions of the underflow concentration, sludge blanket level under unusual conditions, for example the wet-weather condition

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(Torfs et al., 2015).

Given the variety of simulation conditions, such as the sludge settleability and compressibility, 1-D settling models are not considered to be universal for all SST systems, and model parameter adjustment based on experiment data, usually referred as model calibration, is usually required for specific SST simulations. The calibration methodology of the hindered-only settling models are well developed, and can be classified into two categories: 1) the conventional approach using hindered settling velocities obtained from multiple batch settling tests; 2) the direct parameter estimation approach by fitting a single batch settling curve (Vanderhasselt and Vanrolleghem, 2000). It is noticeable that the hindered-compression settling models cannot be calibrated straightforwardly following these two approaches because of the inclusion of the additional compression parameters. Several proposed calibration methods require the use of advanced techniques, such as radiotracing, to measure the dynamic concentration distribution during batch settling experiments (Kinnear, 2002; De Clercq et al., 2005; De Clercq et al., 2008), which is beyond the accessibility of most practical application cases (Li and Stenstrom, 2014b; Ramin et al., 2014c). Therefore, to promote the application of the hindered-compression settling model, great efforts are needed to facilitate its calibration. For example Ramin et al. (2014b, 2014c) reported that calibrating the hindered-compression model based on the additional measurement of the batch bottom concentration, beside the batch settling curves, has achieved some degree of success.

The limited observational data of practical batch experiments naturally gives rise to the problem of the poorly identifiable parameters, which means it is difficult to identify a unique set of all parameters used in the hindered-compression models due to possible parameter correlation (Brun et al., 2002; Brockmann et al., 2008). To avoid this problem, it is important to understand the practical identifiability of the model and select a suitable subset of parameters which can be reliably identified by the available experiment measurements (Weijers and Vanrolleghem, 1997; Brun et al., 2001; Ruano et al., 2007).

In the wastewater treatment process modeling field, two alternative approaches have been most used to analysis the parameter identifiability problem. The first method is on the basis of scalar functions calculated from the Fisher Information Matrix (FIM), and the D and mod-E criteria can be used to select the best identifiable parameter subset (Weijers and Vanrolleghem, 1997). The second method developed by Brun et al. (2001) uses a diagnostic regression and focuses on the analysis of parameter interdependency by calculating the collinearity index. Both methods are proven to be efficient in selecting the best identifiable parameter subset from limited experiment measurements (Weijers and Vanrolleghem, 1997; Brun et al., 2001; Ruano et al., 2007; Brockmann et al., 2008). Recently, the Generalized Likelihood Uncertainty Estimation (GLUE) method has also been demonstrated as a reliable alternative for the identifiability analysis of the hindered-compression settling model by Torfs et al. (2013).

Nevertheless, despite the efficiency of the two most used approaches in addressing parameter identifiability problem, they still have drawbacks which may greatly impact the analysis results, at least in the hindered-compression settling model study. Both approaches are based on the calculation of local sensitivity functions for a set of reasonable parameters values within the parameter space, and in most activated sludge model (ASM) identifiability studies, the initial parameter set is determined as default values reported in literature. For example the practical identifiability analysis of ASM2d by Brun et al. (2002) used the default values presented by Henze et al. (1999) as the starting point values. Given the fact that very limited parameter values have been reported in hindered-compression settling model studies, especially those related to the compression rheology, the initial parameter set values cannot be determined by the default value strategy, which implies that the choice of the initial parameter values may significantly impact the parameter identifiability. Beyond that, fixing some parameters, such as the non-influential parameters determined by the local sensitivity analysis, at prior values according to lecture and practical experience can introduce bias to the parameter estimates, which have been reported in pervious investigations (Weijers and Vanrolleghem, 1997; Brun et al., 2001, 2002; Omlin et al., 2001; Brun et al., 2002).

From a practical point of view, the uncertainty analysis of wastewater treatment plant models is particularly important for design and operation decision making, and one of main uncertainty sources is the model input uncertainty, such as characterizing the model parameter values over a reliable range to reflect the limited knowledge of their exact values (Sin et al., 2009). To facilitate the practical application of the hindered-compression settling models by providing a guidance for experiment design, it is important to know which parameters can be obtained under what experimental conditions, and how large the model prediction uncertainties can be. This knowledge can be very beneficial in understanding the uncertainties of SST performance, such as the sludge blanket height (SBH), the recycle solids concentration under wet-weather and sludge settleability deterioration conditions.

The first objective of this paper is to evaluate the parameter identifiability of the hindered-compression model based on different experimental layouts to show which parameter is identifiable in which experimental layout, as well as to study the influence of initial parameter selection on parameter identifiability analysis. The second goal of this paper aims to investigate the influence of the choice of initial parameter values on parameter identifiability and the bias of the parameter estimates caused by fixing unidentifiable parameters. The third part focuses on the model prediction uncertainty analysis by showing how the estimates obtained from different layouts impact the model prediction uncertainty.

2. Materials and methods

2.1. Model structure

Although having a similar rheological basis, most established hindered-compression models can be distinguished by their modeling approach of the compression settling process (Li and Stenstrom, 2014b). In this study, we selected the recently presented Bürger–Diehl model (no hydrodynamic dispersion considered) as an example for identifiability and uncertainty analysis because of its flexibility in application and available implementation details (Bürger et al., 2011, 2013). The frame of the Bürger-Diehl model can be expressed as eq. (1):

$$\frac{\partial C}{\partial t}+\frac{\partial}{\partial x}F(C,x,t)=\frac{\partial}{\partial x}\left(d_{comp}(C)\frac{\partial C}{\partial x}\right)+\frac{Q_f(t)C_f(t)}{A}\delta(t) \tag{1}$$

where C is the solids concentration, t is time, x is deep from the SST bottom, d_{comp} is the compression function, A is SST surface area, Q_f is the feed flow rate, C_f is the feed solids concentration, δ is the Dirac delta distribution, and the solids transport flux F can be written as eq. (2):

$$F(C,x,t) = \begin{cases} -\frac{Q_e}{A}C_e & effluent\ \ region \\ v_{hs}(C)C - \frac{Q_e}{A}C & clarification\ \ zone \\ v_{hs}(C)C + \frac{Q_u}{A}C & thickening\ \ zone \\ \frac{Q_u}{A}C_u & underflow\ \ region \end{cases} \tag{2}$$

where Q_e is the effluent flow rate, Q_u is the underflow rate, C_e is the effluent solids concentration, C_u is the underflow solids concentration, and v_{hs} is the hindered settling velocity calculated by the Vesilind equation (Vesilind, 1968), shown as eq. (3):

$$v_{hs} = v_0 \exp(-r_h C) \tag{3}$$

The compression function, eq. (4), is derived by Bürger et al. (2012, 2013) which based on the logarithmic compression stress function developed by De Clercq et al. (2008):

$$d_{comp}(C) = \begin{cases} 0 & 0 \le C < C_g \\ \dfrac{\rho_s \cdot \alpha \cdot v_{hs}(C)}{g\left(\rho_s - \rho_f\right)(\beta + C - C_g)} & C \ge C_g \end{cases} \tag{4}$$

where α and β are the compression parameters, and C_g denotes the gel concentration (the threshold compression concentration). Recently, Ramin et al. (2014c) found that the logarithmic compression stress function, as the state-of-the-art function, is not effective for model calibration, even if the additional concentration profile measurements are provided, which implies the need of more accurate mathematical description of the compression behavior.

2.2. Experimental layouts

Currently in both academic research and practical application, the calibration of advanced settling models strongly relies on batch settling measurements, which remains labor intensive and information limited. The lack of high resolution data sets, especially those outside the hindered settling range, greatly challenges the model advancement test and application. Kinnear's data set (Kinnear, 2002) is one of few published data sets that contain both the batch settling curves and concentration profile measurements, which implies it can be used for a comprehensive model performance evaluation. In this study, we select the Salt Lake City Water Reclamation Plant (SLCWRP) subset of the Kinnear's data set, and design four modeling scenarios with increasing difficulty of data collection, as shown in Table 1, to evaluate the influence of experimental layouts on the analysis of parameter identifiability and prediction uncertainty. Since there is no information about the possible measurement error available, the measurement error is not considered in this study. For further information about methodology of data collection, the reader is referred to the literature (Kinnear, 2002).

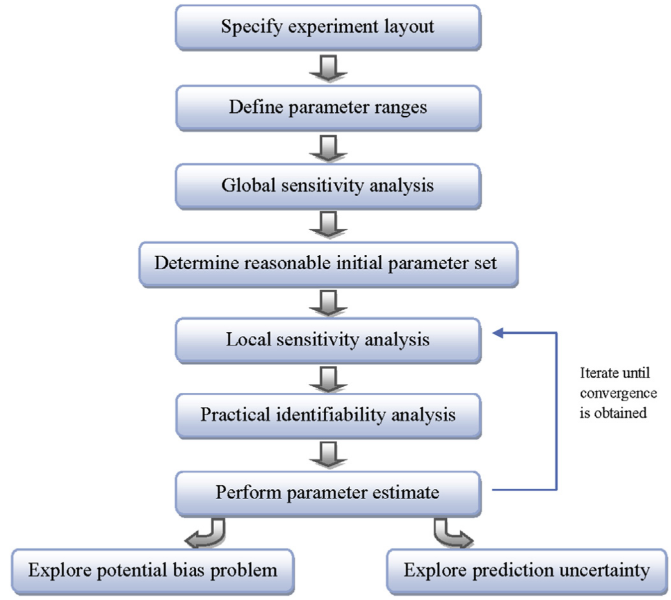

Fig. 1. Steps of a systematic procedure of identifiable parameter subset selection and estimation.

2.3. Identifiability analysis

Fig. 1 shows the procedure for obtaining identifiable parameter subset in different experimental layouts. First, the experimental layout needs to be specified, as shown in Table 1. The proper assessment of prior parameter uncertainties is significant for the subsequent analysis steps, but usually difficult and laborious. The hindered settling parameters (v_0, r_h) are well reported in previous studies (Plósz et al., 2011; Ramin et al., 2014a), while the compression parameters (C_g, α, β) remain poorly understood. Table 2 gives the parameter uncertainties used in this study, which are reasonably estimated based on literature reviews and modeling experience.

By evaluating model outputs which correspond to the experimental data set, the global sensitivity analysis (GSA) has been proved as a reliable approach to preliminarily select the parameter

Table 1
The design of batch settling experiments and comments.

Scenario	Experimental design	Comments
1	Collecting sludge blanket curves with initial concentrations at 1.74, 3.42, 5.46, 8.25, 8.95 kg/m^3 (119 data points);	The sludge blanket curve data is most often collected in batch settling measurements. The linear part of the curve is informative for Vesilind parameter estimation;
2	Collecting sludge blanket curves with initial concentrations at 1.74, 3.42, 5.46, 8.25, 8.95 kg/m^3, and concentration at the static sediment top at 3.42 kg/m^3 (120 data points);	Theoretically, the solids concentration at the static sediment top equals to the gel concentration, the only physically measurable parameter within the hindered-compression settling model;
3	Collecting solids concentration profile of the static sediment with the initial concentration at 3.42 kg/m^3 (7 data points);	The solids concentration profile of the static sediment is difficultly measurable but highly recommended being collected in proposed hindered-compression calibration strategies;
4	Collecting sludge blanket curves with initial concentrations at 1.74, 3.42, 5.46, 8.25, 8.95 kg/m^3, as well as solids concentration profile of the static sediment with initial concentration at 3.42 kg/m^3 (126 data points);	The most informative data set, which is expected to provide information about both the hindered and compression settlings;

Table 2
Uncertainty of the hindered-compression model parameters.

Symbol	Definition	Uncertainty	Reference
V_0	hindered settling parameter [m/h]	3.47–9.71	Plósz et al., 2011, Ramin et al., 2014a
r_h	hindered settling parameter [m^3/kg]	0.15–0.63	Plósz et al., 2011, Ramin et al., 2014a
C_g	Gel concentration [kg/m^3]	5.06–15.27	Kinnear 2002
α	compression settling parameter [Pa]	0–20	De Clercq et al., 2008, Bürger et al., 2013
β	compression settling parameter [kg/m^3]	1–10	De Clercq et al., 2008, Bürger et al., 2013

subset which can be reasonably estimated based on the available information content (Brockmann et al., 2008). Compared with the expert knowledge approach recommended by Brun et al. (2002), GSA is expected to be more objective by considering the whole range of uncertainty of each parameter, and allocating model output uncertainties to the parameter uncertainties (Saltelli et al., 2004). The GSA is carried out by the extended-Fourier Amplitude Testing (e-FAST), originally developed by Cukier et al. (1973) and Schaibly and Shuler (1973), and later extended by Saltelli et al. (1999). As a variance based technique, the e-FAST has its root in the general theorem that the total variance can be decomposed into conditional variances, as shown in eq. (5):

$$Var(sy) = Var(E(sy|\theta_i)) + E(Var(sy|\theta_i)) \tag{5}$$

where *Var* and *E* is the variance and expectancy operator respectively, *sy* denotes a vector of scalar values for the model output and θ_i is the *i*th model factor. The Extended-FAST implementation strategy used in this study is based on Saltelli et al. (1999), and the transformation function is given by eq. (6):

$$\theta_i = \frac{1}{2} + \frac{1}{\pi}\arcsin(\sin(\omega_i s + \varphi_i)) \tag{6}$$

where *s* ranges from $-\pi/2$ to $\pi/2$, w_i is a set of different frequencies and φ_i is a random phase-shift. The total number of model evaluation required can be determined by:

$$N_s = m(2M\omega_{\max} + 1) \tag{7}$$

where *m* is the number of factors, *M* is the interference frequencies, and w_{max} is the maximum frequency. In this study, *M* and ω_{max} is 4 and 8 respectively. For further information about Extended-FAST implementation strategy, such as the selection of ω, the reader is referred to the literature (Saltelli et al., 1999).

Technically, the e-FAST is able to provide two kinds of sensitivity measures: $S_{i,}$ which does not consider the interaction among factors, and S_{Ti}, which accounts for the total contribution of the factor to the output variance. According to Cosenza et al. (2014), S_{Ti} is more informative for determining non-influential factors. Therefore, the global mean sensitivity ($\delta_j^{G,msqr}$) of the model output to the change in θ_j is calculated by:

$$\delta_j^{G,msqr} = \sqrt{\frac{1}{n}\sum_{k=1}^{n}(S_{Ti})^2} \tag{8}$$

where *n* is number of observations. A large $\delta_j^{G,msqr}$ indicates the parameter θ_j is influential to the overall model outputs, and only parameters with $\delta_j^{G,msqr}$ larger than 0.1 are considered to be influential in this study. Given that the global sensitivity measures quantify the averaged influence of parameters on the model outputs, it may not be able to accurately reflect the parameter importance at specific local points, especially for those having global mean sensitivity measures close to the critical value. Therefore, the local mean sensitivity measures, which can calculated by Eq. (9), are used as a supplement to further evaluate the significance of parameters.

As mentioned above, selecting the suitable value of initial parameter set remains a challenge due to the insufficient prior knowledge of biomass settleability and compressibility, as well as the limited number of reported parameter values. The parameters that cannot be reasonably estimated are fixed as the values reported by De Clercq et al. (2008) and Bürger et al. (2013). For the influential parameters, the initial hindered parameter values can be estimated by the conventional hindered settling velocity approach if batch settling curve observations are available, such as in experimental layouts 1, 2 and 4. The initial value of gel concentration (C_g) can be approximated by the concentration at the static sediment top, such as in experimental layouts 2, 3 and 4. Otherwise, the initial influential parameter values are determined by artificial manipulation until an acceptable fit to the experimental observations is obtained.

Parameter identifiability is investigated using the approach proposed by Brun et al. (2001), which is based on the collinearity calculation of the scaled local sensitivity functions ($s_{k,j}$), shown as Eq. (9):

$$s_{k,j} = \frac{\Delta\theta_j}{sc_k}\frac{\partial sy_k}{\partial\theta_j} \quad and \quad \tilde{s}_{k,j} = \frac{s_{k,j}}{\|s_j\|} \tag{9}$$

where $\partial sy_k/\partial\theta_j$ denotes the absolute local sensitivity of model output sy_k to the parameter θ_j; $\Delta\theta_j$ and sc_k are two scale factors which denote the prior uncertainty range of the parameter θ_j and the typical magnitude of the corresponding observations respectively. $\|s_j\|$ is the Euclidean norm of the *j*th column of *S* ($S = \{s_{k,j}\}$). The perturbation factor used is 5%, which is found to be suitable for all the model parameters.

Poor parameter identifiability can be caused by a small sensitivity of the model output to the parameter, or by a high linear dependence of local sensitivity functions (Reichert and Vanrolleghem, 2001). The significance of parameters is determined by the local mean sensitivity function$\delta_j^{L,msqr}$:

$$\delta_j^{L,msqr} = \sqrt{\frac{1}{n}\sum_{k=1}^{n}\left(s_{k,j}\right)^2} \tag{10}$$

The collinearity index is defined as eq. (11) to evaluate the linear dependence:

$$\gamma_k = \frac{1}{\min_{\|\beta=1\|}\left\|\tilde{S}\eta\right\|} = \frac{1}{\sqrt{\min\left(EV\left[\tilde{S}^T\tilde{S}\right]\right)}} \tag{11}$$

where $\tilde{S} = \{\tilde{s}_{k,j}\}$, η is the vector of coefficients, and *EV* denotes the eigenvalue of $[\tilde{S}^T\tilde{S}]$. A large γ_k indicates that the sensitivity functions are highly linearly dependent, which means the changes of model outputs caused by a small change of parameters, such as θ_j, can be mostly compensated by the change of other parameters (Brun et al., 2002). In this study, the parameter subset is considered to be poorly identifiable, if the corresponding γ_k exceeds 10, the threshold recommended by Brun et al. (2001).

To combine the information of the collinearity index and the local sensitivity function, the determinant measure ρ_k is defined as eq. (12), which can be useful in parameter identifiability comparison of different parameter subsets (Brun et al., 2002).

$$\rho_N = \det\left(S_N^T S_N\right)^{1/(2N)} \tag{12}$$

where *det( )* is the determinant function, and N is the number of parameters in the corresponding subset. Since the value of ρ_N strongly depends on the choice of $\Delta\theta_j$, ρ_N is a relative measure suited for comparison of parameter identifiability of different subsets, and cannot be simply evaluated based on an absolute threshold value (Brun et al., 2002). The large $\delta_j^{L,msqr}$ and small γ_k result a large ρ_N, which indicates a good identifiability.

Based on the parameter identifiability analysis results, the parameter estimation is performed by minimizing the weighted residual sum of squares (WRSS):

$$WRSS = (Y - sy(\boldsymbol{\theta}))^T W (Y - sy(\boldsymbol{\theta})) \tag{13}$$

where Y is the experimental observation vector, $\boldsymbol{\theta}$ is the parameter vector, and $W = diag(1/sc_1^2, 1/sc_2^2, \cdots 1/sc_j^2, \cdots 1/sc_M^2)$ is a diagonal weighting matrix. The parameter identifiability analysis and estimation are repeated until convergence is achieved. Since the collinearity measures are calculated based on local sensitivity measures, steps (local sensitivity analysis, practical identifiability analysis, perform parameter estimate) have to be redone after adjusting the initial parameter values, until the convergence of estimates is achieved.

The selection of initial parameter values can profoundly impact the local sensitivity measures, thus potentially influencing parameter identifiability for nonlinear systems (Weijers and Vanrolleghem, 1997). In this study, the influence of initial values selection on parameter identifiability is evaluated based on the approach developed by Brockmann et al. (2008) by using experimental layouts 3 and 4 as examples. Parameters are sampled 800 times over the entire uncertainty space using Latin hypercube sampling, and the corresponding WRSS values are calculated. Only the sampled parameter sets with WRSS smaller than 25 percentile of the total calculated WRSS are considered to provide acceptable predictions and used to investigate the influence of selecting initial parameter values on parameter identifiability.

2.4. Exploring the estimate bias and model prediction uncertainty

In most cases, estimating identifiable parameter subsets from insufficient experimental observations are conditional on the values of prior fixed parameter, which may lead to biased estimates (Brun et al., 2002). To evaluate the influence of the values of fixed parameters on estimates, we reestimate the parameter subset by varying β in the entire prior uncertainty space in layouts 3 and 4.

It is also interesting to investigate the maximum possible model prediction uncertainty reduction if the identifiable parameter subsets are reliably estimated. The prediction uncertainty analysis involves the following steps recommended by Sin et al. (2009):

(1) Specifying input uncertainty: because of the reliable estimation of identifiable parameters, the only uncertainty source is the non-identifiable parameters, and their uncertainty has been shown in Table 2;
(2) Sampling input uncertainty: Latin hypercube sampling strategy is applied;
(3) Propagating input uncertainty to obtain prediction uncertainty: Monte Carlo simulation is applied;
(4) Representation and interpretation of results: the prediction certainty results are represented using mean and percentiles.

3. Results and discussion

3.1. Parameter selection for identifiability analysis

The global sensitivity functions of the four experimental layouts are shown in Table 3. Compared with layout 1, the additional measurement of the top concentration of the static sediment in layout 2, provides a good initial approximation of the gel concentration, but does not impact the sensitivity functions calculation. Hence, the global sensitivity functions of the experimental layouts 1 and 2 are identical. When only the batch settling curve observations are available, such as in experimental layouts 1 and 2, the hindered settling parameters are much more influential than the compression parameters. The large difference of sensitivity functions between hindered and compression parameters may be attributed to the fact that the duration of most batch settling experiments, usually 0.5–1 h, is sufficient to collect hindered settling velocities, but not long enough to obtain compression settling behavior. This implies that calibration approaches based solely on batch settling curves need to be used with caution for hindered-compression model calibration. When concentration profile observations are available, compression parameter sensitivities greatly increase, especially in experimental layout 3, where sensitivity functions of several compression parameters can be even larger than those of hindered settling parameters. This finding shows that the solids concentration distribution in the high concentration range is profoundly influenced by the compression settling behavior, thus making the concentration profile measurements informative for compression parameter calibration, which agrees with the previous conclusion that collecting concentration profile data is recommended for hindered-compression model calibration (Kinnear, 2002; De Clercq et al., 2008; Ramin et al., 2014c).

Initial parameter values as well as the corresponding local mean sensitivity measures, are also shown in Table 3. The important parameters found by the local measures are almost identical to those determined by the global measures, with only one exception: layout 4 where the global and local sensitivity measures cannot reach a consensus of the importance of β. This demonstrates that global sensitivity analysis is reliable for preliminary selection of important parameters, and local sensitivity analysis is also necessary to further evaluate the parameter selection. The influence of selecting initial parameter values to the local sensitivities is also obtained: the change of initial values of C_g and α from 6.00 to 0.31 in experimental layout 1 to 11.06 and 1.94 in experimental layout 2 impact local sensitivities, such as 0.129 changes to 0.213 for C_g. It demonstrates that a proper assessment of initial parameter values is particularly important for identifiability analysis if the available knowledge of model parameter values is limited.

3.2. Parameter identifiability analysis and parameter estimation

To be identifiable, a parameter subset is expected to satisfy two criteria: 1) parameters within the parameter subset must be sufficiently sensitive, which means their local mean sensitivity functions need to be larger than 0.1; 2) the local sensitivity functions of the parameter subset cannot be approximately linearly dependent, and this point is addressed by setting a maximum of the collinearity index as 10. Only if parameter subsets fulfill both criteria, those having high determinant measures are considered to be best

Table 3
Initial values, global and local mean sensitivity measures of the model parameters of layouts 1–4.

Parameter	Layout 1			Layout 2			Layout 3			Layout 4		
	θ^{ini}	$\delta^{G,msqr}$	$\delta^{L,msqr}$	θ^{ini}	$\delta^{G,msqr}$	$\delta^{L,msqr}$	θ^{ini}	$\delta^{G,msqr}$	$\delta^{L,msqr}$	θ^{ini}	$\delta^{G,msqr}$	$\delta^{L,msqr}$
V_0	7.61	0.235	0.421	7.61	0.235	0.487	9.18	0.159	0.107	7.61	0.208	0.506
r_h	0.34	0.815	0.681	0.34	0.815	0.699	0.38	0.245	0.675	0.34	0.701	0.997
C_g	6.00	0.214	0.129	11.06	0.214	0.213	11.06	0.735	0.332	11.06	0.322	0.398
α	0.31	0.168	0.145	1.94	0.168	0.136	0.617	0.271	0.136	0.38	0.146	0.214
β	4.00	0.029	0.056	4.00	0.029	0.011	4.72	0.158	0.103	2.10	0.079	0.119

identifiable.

The collinearity indices and determinant measures of parameter subsets are shown in Table 4. For layouts 1 and 2, all parameter subsets comprising influential parameters are identifiable with collinearity measures as low as 1.00, which means almost no interdependency exists. It is interesting to learn that although in previous studies, batch settling curves (experimental layout 1 and 2) were usually considered to be less informative for calibrating the compression parameters, weak interdependency exists between compression parameters C_g and α. In contrast, parameter subsets including the hindered parameters have a relatively stronger interdependency as their collinearity measures is more than 2. Combining hindered settling parameters (V_0, r_h) and compression settling parameters (C_g and α) does not deteriorate the parameter identifiability. Therefore, parameter subset $\{V_0, r_h, C_g, \alpha\}$ is used for parameter estimation due to its acceptable identifiability.

For experimental layout 3, even though all parameter subsets of size 2 are identifiable with collinearity measures less than 10, subset $\{\alpha, \beta\}$ shows a strong interdependency as its collinearity index is close to the critical value. As expected, parameter subsets comprising $\{\alpha, \beta\}$ are clearly unidentifiable with collinearity measures larger than 10. It is noticeable that although the concentration profile observations are informative for both hindered and compression parameter calibration, simultaneously estimating all parameters is unlikely to be successful based upon the initial parameter selection as shown in Table 3, and the maximum size of identifiable parameter subsets is found to be 3. Consequently, parameter subset $\{r_h, C_g, \alpha\}$ is selected for estimation due to its low collinearity measure ($\gamma = 2.86$) and high determinant measure ($\rho = 0.738$).

With respect to layout 4, the parameter subsets comprising $\{\alpha, \beta\}$ are poorly identifiable as well. Nevertheless, in contrast to layout 3 where no parameter subsets with size more than 3 are identifiable, two subsets of size 4, $\{V_0, r_h, C_g, \alpha\}$ and $\{V_0, r_h, C_g, \beta\}$, are clearly identifiable in layout 4. The comparison of the determinant measures of $\{V_0, r_h, C_g, \alpha\}$ and $\{V_0, r_h, C_g, \beta\}$ shows that the former one is more promising for further evaluation.

Parameter estimation is performed based on the parameter identifiability analysis, and Table 5 summarizes the estimation results and the corresponding correlation matrix information. The low absolute off-diagonal elements of correlation matrixes of all experimental layouts confirm the conditional identifiability of the selected parameter subsets. Estimates of hindered parameters (V_0, r_h) and gel concentration (C_g) differ only slightly from their corresponding initial values, and in contrast, the difference between final estimates and initial values of α can be as large as 30–60%.

To compare the sludge settling properties characterized by the parameter estimates obtained from different experimental layouts, the batch settling flux and compressive solids stress which reflect the sludge settleability and compressibility respectively are

Table 4
Collinearity indices and determinant measures of parameter subsets of experimental layouts 1–4.

Set number	Parameters	Layout 1		Layout 2		Layout 3		Layout 4	
		γ_k	ρ_k	γ_k	ρ_k	γ_k	ρ_k	γ_k	ρ_k
1	V_0, r_h	2.23	0.775	2.67	0.714	3.67	0.615	2.21	0.779
2	V_0, C_g	1.22	0.972	1.01	1.00	1.18	0.979	1.25	0.967
3	V_0, α	1.00	1.00	1.00	1.00	1.63	0.884	2.24	0.968
4	V_0, β	–	–	–	–	1.45	0.923	1.24	0.968
5	r_h, C_g	1.21	0.975	1.05	0.998	1.36	0.943	1.81	0.850
6	r_h, α	1.19	0.978	1.11	0.991	1.63	0.884	1.81	0.848
7	r_h, β	–	–	–	–	1.52	0.908	1.80	0.849
8	C_g, α	1.00	1.00	1.00	1.00	2.59	0.724	4.78	0.541
9	C_g, β	–	–	–	–	3.43	0.635	5.31	0.514
10	α, β	–	–	–	–	9.21	0.391	**26.1**	0.233
11	V_0, r_h, C_g	2.23	0.827	2.71	0.797	4.23	0.675	3.08	0.732
12	V_0, r_h, α	2.59	0.806	2.91	0.778	3.67	0.663	3.14	0.728
13	V_0, r_h, β	–	–	–	–	3.71	0.678	3.14	0.729
14	V_0, C_g, α	1.22	0.981	1.01	0.999	3.88	0.689	4.78	0.649
15	V_0, C_g, β	–	–	–	–	4.52	0.658	5.32	0.627
16	V_0, α, β	–	–	–	–	**15.9**	0.418	**26.2**	0.370
17	r_h, C_g, α	1.32	0.967	1.13	0.992	2.86	0.738	4.78	0.593
18	r_h, C_g, β	–	–	–	–	3.63	0.689	5.31	0.574
19	r_h, α, β	–	–	–	–	**10.6**	0.476	**26.2**	0.339
20	C_g, α, β	–	–	–	–	**20.8**	0.319	**31.7**	0.232
21	V_0, r_h, C_g, α	2.59	0.838	2.94	0.826	**12.2**	0.481	4.79	0.578
22	V_0, r_h, C_g, β	–	–	–	–	**11.6**	0.476	5.33	0.564
23	V_0, r_h, α, β	–	–	–	–	**33.7**	0.339	**26.2**	0.380
24	V_0, C_g, α, β	–	–	–	–	**32.7**	0.340	**31.9**	0.328
25	r_h, C_g, α, β	–	–	–	–	**28.9**	0.367	**32.1**	0.306
26	V_0, r_h, C_g, α, β	–	–	–	–	**36.5**	0.289	**32.1**	0.342

*Collinearity indices larger than 10 are in bold.

Table 5
Initial values, final estimates, standard errors and correlation matrixes of the parameter subsets selected in experimental layouts 1–4.

Experiment layout 1

Parameter	θ^{est}	Standard error		Correlation matrix			
		Absolute	Relative	V_0	r_h	C_g	α
V_0	7.41	0.072	0.009	1			
r_h	0.34	0.004	0.011	0.446	1		
C_g	6.46	0.549	0.085	0.053	−0.081	1	
α	0.22	0.028	0.127	−0.042	−0.297	0.084	1

Experiment layout 2

Parameter	θ^{est}	Standard error		Correlation matrix			
		Absolute	Relative	V_0	r_h	C_g	α
V_0	6.99	0.098	0.014	1			
r_h	0.33	0.004	0.013	0.538	1		
C_g	11.8	0.196	0.017	0.356	−0.007	1	
α	1.01	0.086	0.085	0.100	−0.039	0.018	1

Experiment layout 3

Parameter	θ^{est}	Standard error		Correlation matrix		
		Absolute	Relative	r_h	C_g	α
r_h	0.33	0.015	0.045	1		
C_g	10.51	0.866	0.082	−0.424	1	
α	0.82	0.109	0.133	0.406	0.838	1

Experiment layout 4

Parameter	θ^{est}	Standard error		Correlation matrix			
		Absolute	Relative	V_0	r_h	C_g	α
V_0	6.98	0.096	0.014	1			
r_h	0.34	0.004	0.011	0.542	1		
C_g	10.7	0.177	0.017	0.376	0.405	1	
α	0.39	0.433	0.111	−0.121	−0.408	−0.428	1

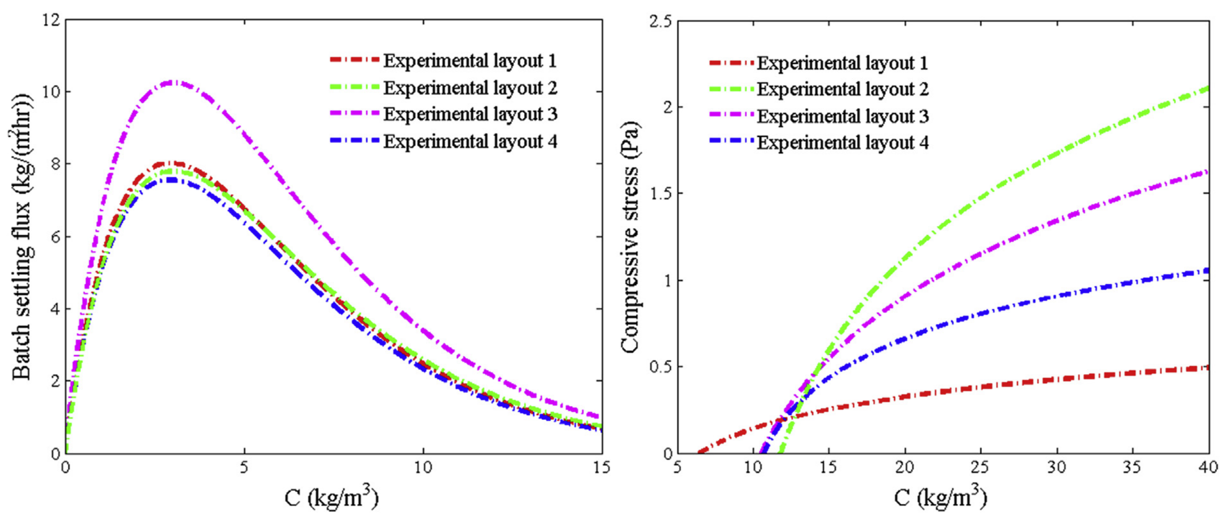

Fig. 2. The estimated batch settling flux functions (left) and compressive stress functions (right) calculated based on the Vesilind equation (Vesilind, 1968) and the logarithmic compression stress equation (De Clercq et al., 2008).

calculated and shown in Fig. 2. The estimated settling fluxes are similar or identical with only one notable exception: the batch flux of layout 3, which implies a better sludge settleability, especially in medium and high concentration range. This discrepancy possibly can be caused by the difference in obtaining initial hindered parameter values; the same initial values of hindered parameters are used in layout 1, 2 and 4 which are determined by the conventional hindered settling velocity approach. In layout 3 where no batch settling curve observations are available, the initial values of the hindered settling parameters are selected by experience or manual parameter adjustment. Fig. 2 also shows that the estimated sludge compressibility characterized by compressive solids stress curves of different layouts are inconsistent, which is mostly reflected by the difference of estimated gel concentrations and magnitude of effective solids stress. The effective solids stress curve estimated in experimental layout 1 possesses the smallest gel concentration and magnitude, which is consistent with the smallest initial values of *Cg* and α used in this case as compared with other layouts. Estimated effective solids stress curves of layout 2, 3 and 4 are similar in gel concentration, but greatly differ in stress magnitude, which can be attributed to the fact that in these layouts, similar gel concentration estimates but different α estimates are obtained.

To facilitate an understanding of the limitations of each layout in model calibration, we compare model simulations based on parameter estimates of layouts 1–4 to complete experiment observations (batch settling curves and concentration profiles), shown in Fig. 3. As expected, model simulations based on estimates obtained in layout 4 fit well with both batch settling curves and concentration profiles. Simulations of layout 3 provide the best fit with concentration profile observations, while the predicted batch settling curves are much lower than experiment observations, which implies that the estimated batch settling flux of layout 3 cannot represent real sludge settleability. Accurate predictions of static concentration profiles in layout 3 may be achieved by overestimating the sludge settleability while underestimating its compressibility. Therefore, estimating sludge settleability and compressibility by only using static concentration observations, such as experimental layout 3, may be questionable. Simulations of layout 1 and 2 provide fairly good fits to observed batch settling curves. Simulations of layout 1 slightly overestimate batch settling curves of 8.25, 8.95 kg/m^3, which may be caused by the underestimated gel concentration. Although simulations based upon layout 2 succeed in predicting the top concentration of static sediment, the predicted concentration within the sediment is lower than the experiment observations due to the relatively large

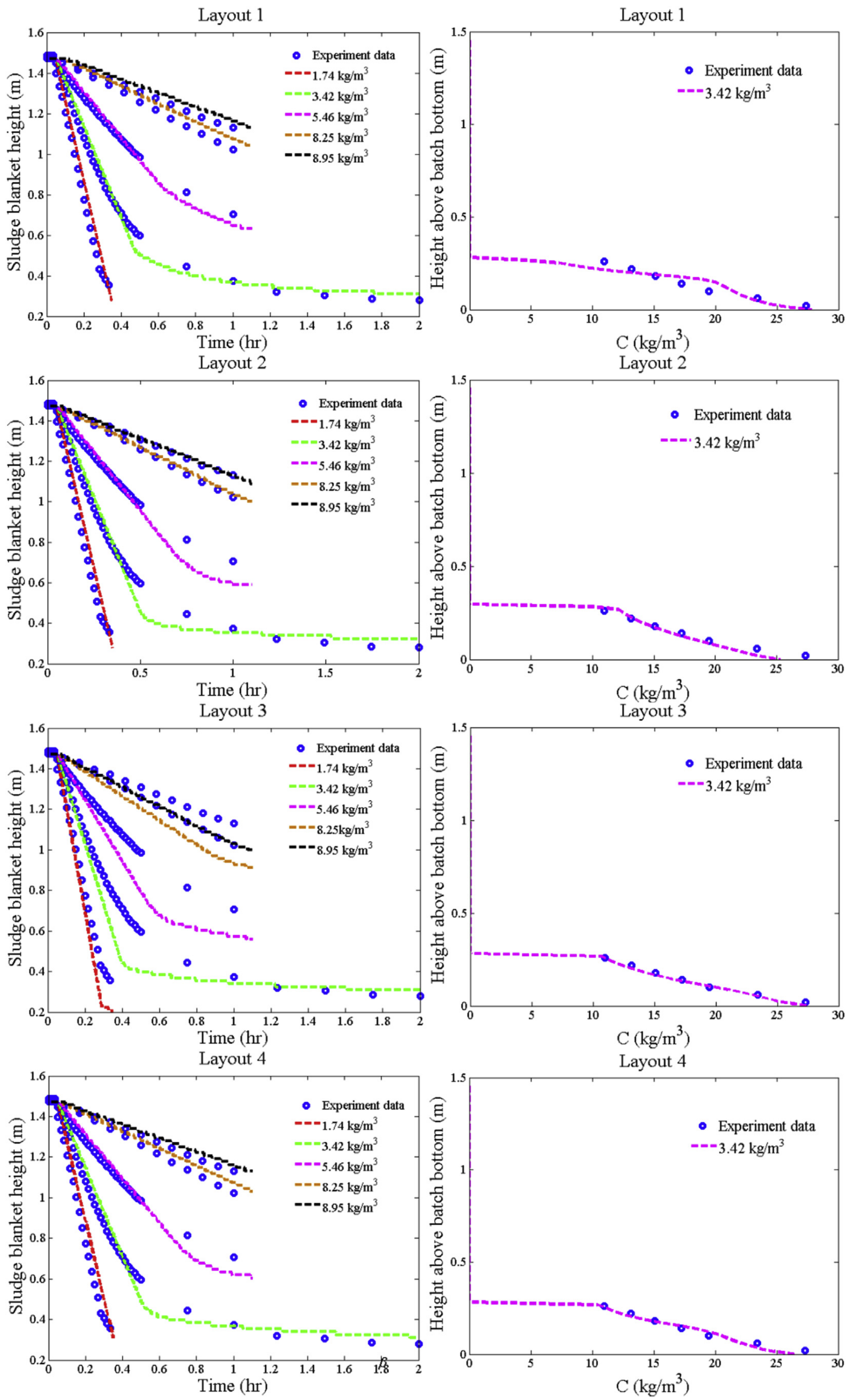

Fig. 3. Simulation results (batch settling curves and concentration profile) based on parameter subset estimations of experiment layouts 1–4.

estimated compressive solids stress as shown in Fig. 2. Consequently, accurately estimating compressibility remains a challenge if using only batch settling curve observations.

3.3. Influence of selecting initial parameter values on parameter identifiability

The selection of parameter initial values impacts parameter identifiability in two ways: 1) impact local parameter sensitivity functions; 2) impact collinearity measures of parameter subsets. If initial values of C_g and hindered parameters are determined by measuring the top concentration of static sediment and hindered settling velocities respectively, the sensitivity analysis of parameter identifiability to initial parameter selection only needs to consider the remaining parameters (V_0, r_h, α, β in experimental layout 3, and α, β in experimental layout 4), which may have different initial values.

Fig. 4 shows the change of local mean sensitivity functions with different initial parameter values. For experimental layout 3, changes of parameter initial values mostly influence the local mean sensitivity functions of V_0, r_h α and β. In spite of the variance of sensitivity functions, the gel concentration, C_g, remains influential as its 25% percentile is above the critical value defined as 0.1 in this study. Fig. 4 also shows that compared with other parameters, C_g possesses the highest median of the local mean sensitivity functions, which agrees with the global sensitivity analysis conclusion that C_g is the most influential parameter in layout 3. In layout 4, the hindered settling parameters, V_0 and r_h, are the most influential parameters, and their sensitivity functions are almost insensitive to the initial value changes of α and β. Even though a moderate variance of the sensitivity measures of C_g is observed, it remains as a significant parameter with 5th percentile above the critical value. The only potentially non-influential parameters are α and β, whose 75th percentiles are close to the critical value.

Box–Whisker plots for collinearity indices of parameter subsets calculated based on sampled parameters are shown in Fig. 5. For experimental layout 3, the parameter subsets of size 2 are mostly identifiable, and their collinearity measures are not sensitive to the change of initial parameter values. Poor identifiability only can be obtained in subsets 1 {V_0, r_h} and 10 {α, β} for their median and 75 percentile are above the critical value. This implies that parameter subsets comprising {V_0, r_h} or {α, β} can be less identifiable than others. For subsets of size 3 and 4, the increase of parameter subset size leads to the variation of collinearity measures as well as the deterioration of identifiability, with only one notable exception: subset 14 {r_h, C_g, α}, which is clearly identifiable independently of change of initial parameter values. This agrees well with the conclusion that parameter subsets that do not include {V_0, r_h} or {α, β} show a better identifiability. Subset 26 {V_0, r_h, C_g, α, β} is poorly identifiable as the 5th percentile is above the critical value, thus making it unreliable for estimating all parameters simultaneously. Compared to layout 3, collinearity measures of parameter subsets of layout 4 are less sensitive to initial parameter value selection. Clearly, most parameter subsets are identifiable regardless of the initial parameter values, and for several of them, for example the subsets of size 2, the collinearity measures are smaller than 1.5, indicating the absence of interdependence. Consequently, for layout 4, the size of parameter set that can be reliably estimated can be as large as 5, if parameters included are found to be influential to the experiment observations.

3.4. Exploring potential bias problem and prediction uncertainty

It is noteworthy that the estimates obtained by identifiable parameter subset estimation are clearly conditional on fixed values of unidentifiable parameters, hence potentially causing estimate bias problems (Brun et al., 2002). Fig. 6 shows the reestimated results of layouts 3 and 4 using the parameter estimates shown in Table 5 as references, and Table 6 provides the average collinearity measures of all parameter subsets of size 2, composed of one identifiable parameter plus the fixed parameter, and the average estimate change of the corresponding identifiable parameter. As can be seen, the large average change is always associated with the large average collinearity measure, which indicates that the stronger the parameter is correlated to the fixed parameter, the more sensitive the estimate is to the change of the fixed parameter value. For layout 3, the small average collinearity measures of subsets {r_h, β}, {V_0, β} indicate the week interdependency between r_h and β, C_g and β, and as a result, the estimates of the r_h and C_g are almost insensitive to β, which is demonstrated by the low average changes (<10%). However, concerning α, the increase of β leads to a significant increase of α, and the corresponding average change can be as high as 49.7%. The strong sensitivity of the estimate of α to the fixing β can be attributed to the significant interdependency of α and β with average collinearity measure as high as 19, which means that changes in β can be compensated by corresponding changes of α. When it comes to layout 4, almost no interdependency exists in subsets {V_0, β}, {r_h, β} and {C_g, β} as their corresponding average

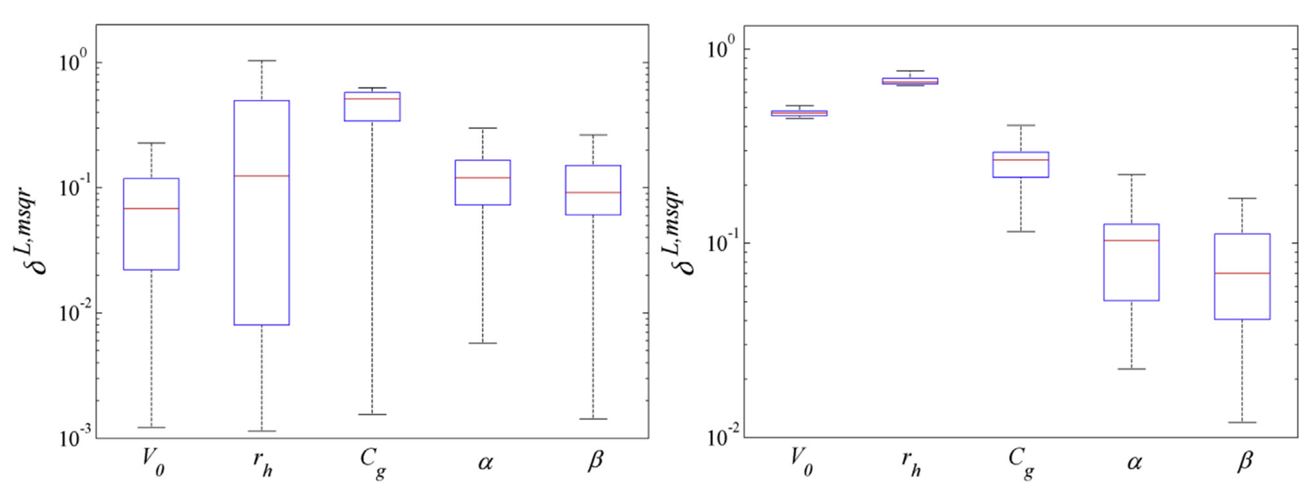

Fig. 4. Box–Whisker plot of the local mean sensitivity measures of model parameters in layouts 3 and 4. The upper and lower boundaries of the box mark the 75th and 25th percentile, and line within the box marks the median. Whiskers above and below indicate the 95th and 5th percentile. (left: experimental layout 3; right: experimental layout 4).

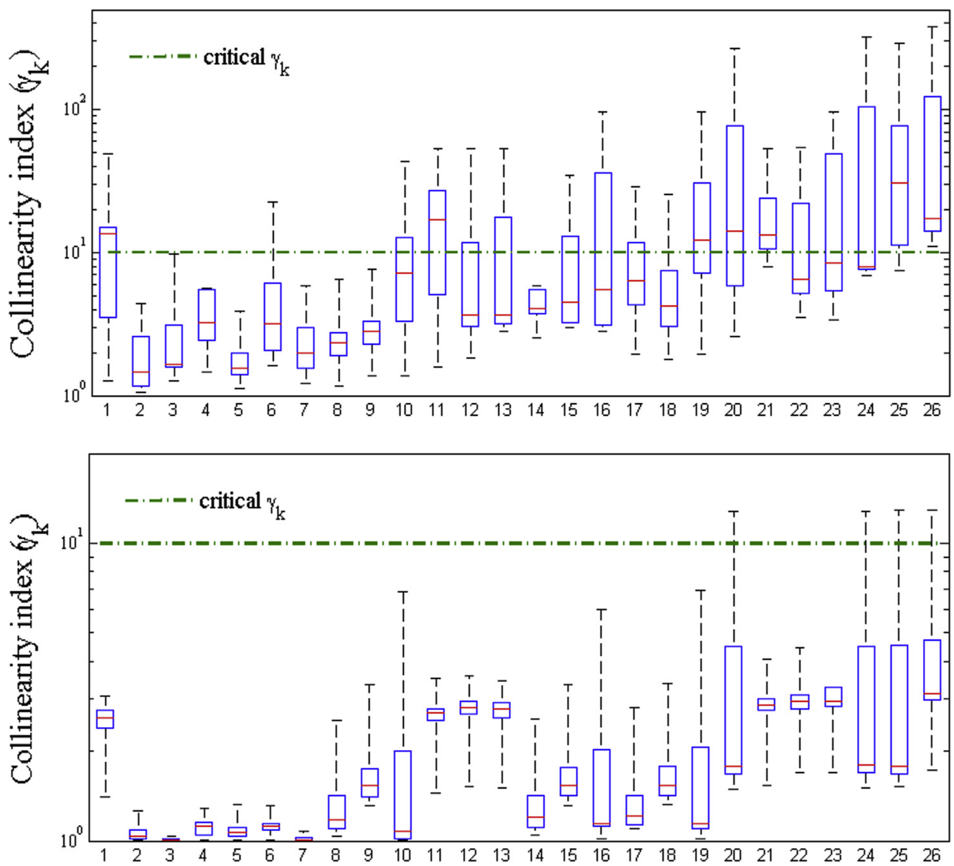

Fig. 5. Box–Whisker plot of the calculated collinearity indices for all parameter subsets of size 2–5. (the order of the parameter subsets is the same as the parameter set number as shown in Table 4). The upper and lower boundaries of the box mark the 75th and 25th percentile, and line within the box marks the median. Whiskers above and below indicate the 95th and 5th percentile. (top: experimental layout 3; bottom: experimental layout 4).

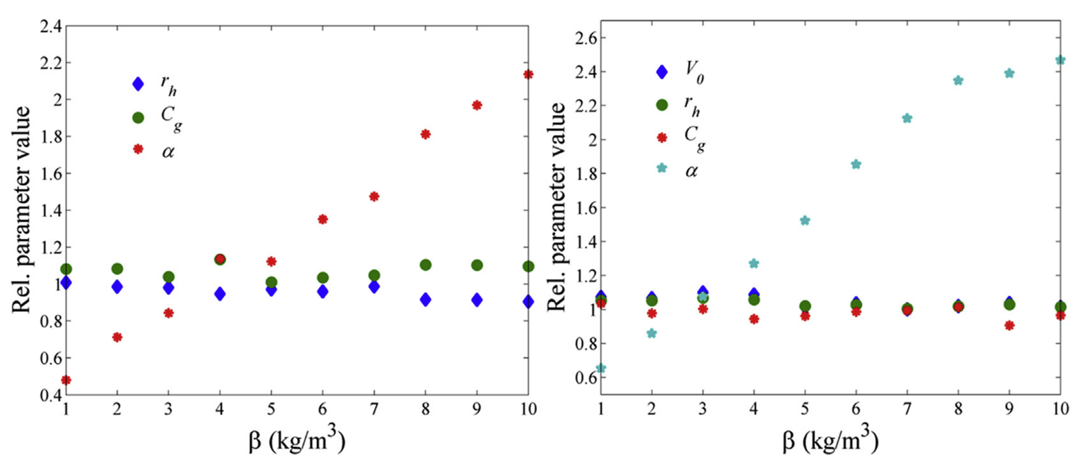

Fig. 6. Relative values of estimated parameter for different values of fixed parameters (left: experimental layout 3; right: experimental layout 4).

Table 6
The average collinearity indices of parameter subsets of size 2 consisting of one identifiable parameter plus the fixed parameter, and the average changes of the estimates of identifiable parameters.

Experimental layout 3			Experimental layout 4		
Parameter	Average γ	Average change (%)	Parameter	Average γ	Average change (%)
r_h	3.13	4.95	V_0	1.15	4.39
C_g	5.41	8.43	r_h	1.31	3.02
α	16.78	49.7	C_g	2.52	3.19
			α	3.10	98.4

collinearity indices approach to 1. Conversely, the collinearity measures of $\{\alpha, \beta\}$ are relatively larger, which leads to poor identifiability problem. Obviously, the estimates of α in layouts 3 and 4 can only be seen as reasonable values which leads to a sufficient description of experiment observations rather than "true parameter value".

To obtain prediction uncertainty of the hindered-compression model, we assume uncorrected parameters with the prior uncertainties as shown in Table 2, and zero uncertainty for the identifiable parameters of each layout. The model prediction uncertainty is calculated by using Latin hypercube sampling and Monte Carlo simulation. We consider the SST with the same configuration as proposed by Bürger et al. (2013), the volumetric flow $Q_u = 80$ m^3/h and Q_f is modeled by the harmonic function developed by Carstensen et al. (1998). The feed concentration is chosen as

$$C_f(t) = \begin{cases} 6 & 0 \le t < 48\ hr \\ 7.5 & 48 \le t < 72\ hr \\ 4 & 72 \le t < 168\ hr \end{cases} \tag{12a}$$

Fig. 7 shows the uncertainty ranges of SBH which is one of the most significant model outputs for system robustness and efficiency analysis. Given that model simulations based on estimation results of layouts 1, 2 and 4 possess the same uncertainty source - the non-identifiable β, it is interesting to compare their corresponding prediction uncertainties. Clearly, after estimating the identifiable parameter subsets of layouts 1, 2 and 4, the model prediction uncertainties become low, and the 5th percentile almost overlaps with the 95th percentile for SBH in layouts 1 and 4. Similar tendencies of SBH are obtained; however the difference in the prediction of peak SBH uncertainties can cause a discrepancy in developing control strategies. For layout 2 and 4, the 5th percentile of peak SBH is above 3 m (the feed inlet), which indicates a high opportunity of thickening failure, and the 95th percentile is close to 4 m (the effluent weir), which implies the potential risk of clarification failure. Hence, in order to avoid failure, a proper operating adjustment is needed from t = 48–72 h, such as increasing the underflow rate. Conversely, for layout 1, since the 95th percentile of peak SBH uncertainty is below 3.5 m, failure is not expected. For layout 3 where two uncertainty sources (V_0 and β) exist, the uncertainty of SBH remains large, which implies that SBH is sensitive to these two parameters. If the unidentifiable parameters characterize the sludge with good settleability and compressibility, the growth of SBH can be moderate as the 5th percentile line shows. However, if the unidentifiable parameters lead to poor settleability and compressibility, a rapid change of SBH is expected as 95th percentile line shows, which can potentially cause thickening and clarification failures. Therefore, further operational adjustments are required to account for the shock increase of the solids flux for layout 3.

4. Conclusion

In this paper, we provide a systematic analysis of model parameter identifiability in different experimental layouts, as well as the influence of selecting initial parameter values on parameter identifiability. Additionally, we further investigate the bias introduced by fixing parameters, and evaluate the model prediction uncertainties based on the estimation of identifiable parameter subsets. Specific conclusions can be made as followings:

- As shown by the global sensitivity results, the hindered settling parameters are more influential in situations where only batch settling curve observations are available, while the sensitivity to compression parameters can be greatly increased if

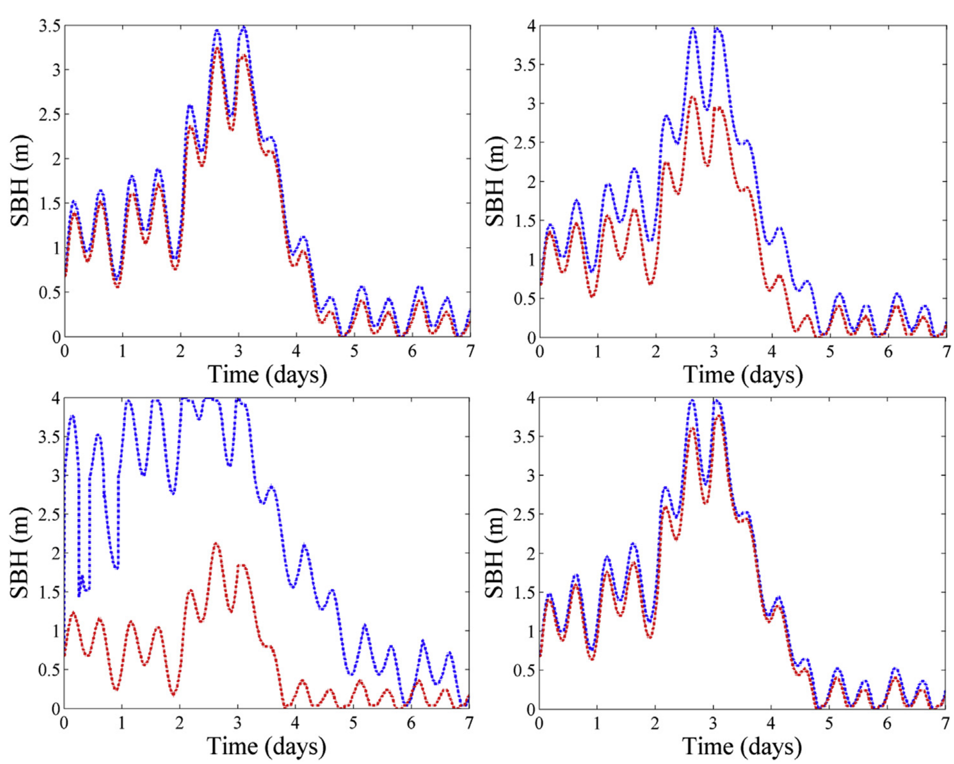

Fig. 7. Uncertainty of SBH based on parameter subset estimation of experimental layout 1–4. The blue and red dot lines indicate the 95th and the 5th percentile respectively. (top left: experimental layout 1; top right: experimental layout 2; bottom left: experimental layout 3; bottom right: experimental layout 4). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

concentration profile observations are included. This supports the previous conclusion that concentration profile observations are informative for compression parameter calibration.

- The identifiability analysis shows that at least three model parameters are conditionally identifiable, and β is most difficult to identify. Parameter estimates obtained from data sets only including the batch settling curves or the concentration profile fail to provide adequate description of the concentration profile observations and batch settling curve observations respectively, which implies the risk of calibrating model by using experimental measurements without sufficient information content.
- Because of the application of local sensitivity functions, the parameter identifiability analysis can be sensitive to the initial parameter value selection. Determining the initial values of the hindered parameters and C_g by measuring the hindered settling velocities and the top concentration of the static sediment respectively is highly recommended to minimize the sensitivity of parameter subset identifiability to the change of initial parameter values.
- Estimates obtained by identifiable parameter subsets estimation are conditional on the values of fixed parameters. For these identifiable parameters, the more correlated they are to fixed parameters, the more sensitive their estimates are to the change of the fixed parameters. Reliably estimating identifiable parameters can reduce the model prediction uncertainty of SBH to some degree. However, in terms of the prediction uncertainty of peak SBH, the uncertainty analysis based on the estimates of different layouts cannot lead to consistent operation strategies, which implies that the hindered-compression continuous settling model cannot be used as quantitative prediction tool if calibrated without comprehensive data measurements.

It is worthy to note that in this study, we investigate the practical identifiability of SST model mostly based on the state-of-the-art settling model, since the prior uncertainty of all parameters in the model are well documented in previous investigations. Currently, several more advanced settling models have been developed to improve the model predictions, for example the hindered-transient-compression model developed by Ramin et al. (2014c) have been demonstrated to be more effective than the state-of-the-art settling model for batch settling predication. For these advanced SST models, the increase of model complexity can be expected, such as the size of model parameters can be close 10. The procedures and techniques used in this study, can also be a reliable framework for the parameter identifiability analysis of these advanced SST models.

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