# Batch settling curve registration via image data modeling

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#### 9 Abstract

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To this day, obtaining reliable characterization of sludge settling properties remains a challenging and time-consuming task. Without such assessments however, optimal design and operation of secondary settling tanks is challenging and conservative approaches will remain necessary. With this study, we show that automated sludge blanket height registration and zone settling velocity estimation is possible thanks to analysis of images taken during batch settling experiments. The experimental setup is particularly interesting for practical applications as it consists of off-the-shelf components only, no moving parts are required, and the software is released publicly. Furthermore, the proposed multivariate shape constrained spline model for image analysis appears to be a promising method for reliable sludge blanket height profile registration.

- 10 Keywords: secondary clarifiers, separation processes, shape constrained
- <sup>11</sup> splines, sludge blanket height, sludge settling, wastewater treatment

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Acronyms	Full expression
AO	Automated, on-line
QR	Qualitative representation
SBH	Sludge blanket height
SCS	Shape constrained splines
VO	Visual, off-line
VS, VS1, VS2	Visual, simultaneous
ZSV	Zone settling velocity

# List of acronyms

List of Symbols.

Symbol	Definition	
$\beta$	All spline function coefficients	
$oldsymbol{eta}_k$	Coefficients of the $k$ th spline function	
$oldsymbol{ heta},\  heta_t$	Transitions ( $t$ th transition)	
Θ	Feasible set for $\boldsymbol{\theta}$	
Ω	Feasible set for $oldsymbol{eta}$	
$\underline{\boldsymbol{b}},\overline{\boldsymbol{b}},\underline{b_e},\overline{b_e}$	Interval boundaries (for episode $e$ )	
d	Derivative index	
e	Episode index	
$f_k$	kth function	
$f_k^{(d)}$	dth derivative of the $k$ th function	
g	Objective function	
j	Pixel index	
$\hat{h}, \ \hat{m{h}}_{AO}, \ \hat{m{h}}_{VO},$	Sludge blanket height (SBH) estimates	
$\hat{m{h}}_{VS1},\hat{m{h}}_{VS2}$	(AO/VO/VS1/VS2: see list of acronyms)	
$h_L,h_U$	Physical height corresponding to the top/bottom (U/L) $$	
	pixel	
i	Image index	
k	Data series index, color channel index	
$r_v$	Parameter of the Vesilind equation	
q	Flux	
$s_{e,d+1}$	Sign for the $d$ th derivative in the $e$ th episode	
u	Integration variable	
v	Settling velocity	

$v_0$	Parameter of the Vesilind equation
$x, x_h$	Pixel position (for the <i>h</i> th row in $\tilde{\boldsymbol{Y}}$ )
$\boldsymbol{x}$	Independent data vector, pixel positions
$z, \boldsymbol{z}_{AO}, \boldsymbol{z}_{VO},$	Sludge blanket height (SBH) sampling times
$oldsymbol{z}_{VS}$	(AO/VO/VS1/VS2: see list of acronyms)
$oldsymbol{B}_k$	Basis matrix for $f_k$
$D_k$	Maximum considered derivative degree for the shape con-
	straints applied to $f_k$
E	Number of episodes
Ι	Number of images in an experiment
J	Number of functions to fit
Н	Number of rows in $ ilde{m{Y}}$
K	Number of data series to approximate, number of color
	channels
$\boldsymbol{S}$	Matrix describing the qualitative sequence, i.e. series of
	primitives
T	Number of transitions
Y	Model estimates
$ ilde{m{Y}}$	Measurement matrix

### 12 1. Introduction

Settling is one of the key processes in activated sludge wastewater treat-13 ment plants (WWTPs, Ekama et al., 1997). Its primary function is the 14 clarification of mixed liquor, thereby preventing wasting organic material 15 and nutrients into the water bodies that receive the treated wastewater. In 16 addition, settling results in the thickening of sludge thereby increasing the 17 efficiency of biological conversion processes occurring in the reactor tanks 18 of the WWTPs. Accurate design of settlers requires a proper characteriza-19 tion of the sludge settling properties. In addition, WWTP operation can be 20 improved by avoiding overloaded settler conditions or increasing the reactor 21 efficiency by (i) manipulation of the recycle flow rate (Balslev et al., 1994; 22 Chen and Beck, 2001; Mines Jr et al., 2001), (ii) step feed (also: step aera-23 tion) and step sludge control (Chen and Beck, 2001), or *(iii)* short-term use 24 of the reactor tanks for sludge sedimentation and storage. Settling also plays 25 an essential role during the primary clarification process. Inefficient removal 26 of suspended solids prior to biological treatment results in higher oxygen 27 demand (for oxidizing organic pollution) and lower biogas production. For 28 innovative technologies, such as granular sludge processes, settling governs 29 the separation of the slow and fast settling biomass, i.e., the selection of the 30 granules and the selective removal of flocs through excess sludge removal. A 31 proper characterization of the settling properties of the sludge is thus nec-32 essary for a variety of separation processes that can be found on small and 33 large WWTPs. 34

Different parameters are available to characterize the sludge settling properties (van Loosdrecht et al., 2016): the sludge volume index (SVI), the di-

luted sludge volume index (DSVI), the stirred specific volume index at 3.5 37 min (SSVI3.5), etc. Unfortunately, such measures provide an incomplete 38 description of the sludge settling properties (van Loosdrecht et al., 2016). 39 A more detailed characterization of the sludge settleability is provided by 40 sludge blanket height (SBH) profiles (van Loosdrecht et al., 2016). However, 41 measuring such profiles is significantly more time-consuming than measuring 42 sludge settling properties (SVI, etc.). Therefore, several empirical corre-43 lations were proposed to link the settling model parameters to the sludge 44 settling measures that are easy to obtain. Such empirical correlations form 45 the basis of today's practice, including control systems (e.g., Traoré et al., 46 2006). and despite known limits reported in several studies (Ozinsky and 47 Ekama, 1995a,b; Bye and Dold, 1998). 48

A dynamic settling model commonly used in today's practice is the expo-49 nential model first proposed in Vesilind (1968). Still, several more detailed 50 models have been built and studied (e.g., Cacossa and Vaccari, 1994; Plósz 51 et al., 2007; Ramin et al., 2014; Li and Stenstrom, 2016). Critical to any 52 study of settling behavior is the collection of SBH profiles registered dur-53 ing batch settling experiments as discussed above. All of the aforementioned 54 studies rely on SBH measurements obtained by visual inspection of a settling 55 column during the batch settling experiments. Typical use of SBH profiles 56 may provide only one data point per experiment, e.g. when the zone settling 57 velocity (ZSV) measurement corresponding to a single total suspended solids 58 concentration is of interest only. As a result, collecting sufficient data to 59 empirically describe the zone settling velocity and flux curves is a cumber-60 some and time-intensive task that can be afforded within research projects 61

but is rarely executed routinely on WWTPs, as already reported in Daig-62 ger and Roper Jr (1985). The potential of the developed settling models 63 for optimization or control of WWTP operation is likely only realized if a 64 routinely applicable yet inexpensive method for SBH registration is avail-65 able. The lack of an easy, quick, and reliable method for the measurement 66 of batch settling curves is still one of the main limitations for both research 67 and practice (Li and Stenstrom, 2014). We therefore focus on the problem 68 of batch settling curve registration yet also demonstrate how the resulting 69 batch settling profiles can be used for dynamic modeling. 70

Devices for automated SBH registration are available today (e.g., Van-71 rolleghem et al., 2006). However, they are likely too expensive to obtain 72 and maintain for routine monitoring purposes. Methods to automate and/or 73 advance SBH registration include (i) light intensity scanning (Vanrolleghem 74 et al., 1996), (ii) measurement of a radioactive tracer (De Clercq et al., 2005), 75 (iii) use of an ultrasonic transducer (Locatelli et al., 2015), and (iv) high-76 speed camera imaging (Mancell-Egala et al., 2016). The applicability of such 77 techniques may remain limited unless (i) on-site use is feasible to avoid ef-78 fects of sample deterioration and (ii) the devices are easy to maintain by 79 technical staff on typical wastewater treatment plants. 80

The main objective of our work is to produce, demonstrate, and validate a novel method for automated image-based SBH registration. Automated sample preparation is considered for future study. The proposed method for batch settling curve registration consists of *(i)* using an inexpensive off-theshelf camera to collect images during multiple batch settling experiments and *(ii)* fitting a shape constrained spline (SCS) model extended for the <sup>87</sup> purpose of image analysis. The main advantage of our method is that the <sup>88</sup> experimental method is accessible to researchers and practitioners as only <sup>89</sup> inexpensive off-the-shelf equipment is used. A side benefit of applying the <sup>90</sup> SCS model is that it enables use of multi-channel data present in the collected <sup>91</sup> images and avoids differentiation of the noisy data during image analysis, in <sup>92</sup> contrast to existing methods (e.g., Kim et al., 2011).

The proposed method exploits knowledge about the expected shape of 93 the light intensity profile along the vertical dimension of the sludge column. 94 Using shape information to characterize settling behavior is not new however. 95 For example, it is known that the SBH profile obtained with conventional 96 batch settling experiments with ideal suspensions is described as a convex 97 profile, corresponding to a convex section of the solids flux curve that gov-98 erns such experiments. Similarly, recently proposed batch experiments de-99 liver concave height profiles governed by concave sections of the solids flux 100 curve. Knowledge about the shape is exploited in Diehl (2007); Bürger and 101 Diehl (2013); Diehl (2015). Our work is different from these historical ap-102 proaches in two ways. First, our method allows fitting functions which have 103 a changing shape along their domain, as opposed to previous work. In our 104 particular study, functions consisting of a concave segment followed by a 105 convex segment are estimated. Secondly, the convex-concave shape enables 106 explicit accounting of non-ideal behavior during experiments. Indeed, we 107 study batch settling experiments where the effects of turbulence at the start 108 of the experiments cannot be ignored. In what follows, the most important 109 aspects of our method and the most significant results are explained. 110

#### 111 2. Materials and Methods

#### 112 2.1. Batch Settling Experiments

Nine batch settling experiments have been executed. Each of the settling 113 experiments is executed for a dilution of a granular sludge sample obtained 114 from a column sequencing batch reactor located at Eawag and fed with low-115 strength municipal wastewater. Two such samples were taken directly from 116 the reactor as source material for diluted sludge sample preparation. The 117 sludge sample index and the applied dilutions for each of the experiments 118 are given in Table 1. The total suspended solids concentration on the day 119 of experimentation was 2.4 g/L. Throughout experimentation, a 2 L vertical 120 glass cylinder is used. Each batch settling experiment was started by filling 121 the glass cylinder with the (diluted) sludge and by ensuring homogeneity at 122 the start of the experiment by means of manual stirring with a glass rod. 123

A scheme of the experimental set up can be seen in Fig. 1. During each 124 experiment, images are taken by means of a digital camera (Camera 1, Canon 125 PowerShot G9) equipped with a continuous power supply and modified with 126 the Canon Hack Development Kit (CHDK, 2016) software to continuously 127 capture images at intervals of 15s. Camera 1 was positioned so that (i)128 the height of the camera corresponds to the top of the sludge column, (ii)129 the central line of sight of the camera is directed at the top of the sludge 130 column and (iii) the complete column is visible in the image. Within each 131 experiment, the images are indexed with  $i \ (i = 1, \dots, I)$ . 132

In experiments 5 and 6, two experimenters (experimenter 1 and 2) registered the SBH by means of visual inspection of the settling sludge column at time intervals of 30s as conventional experimentation (van Loosdrecht et al.,

2016) and as close as possible to every 2nd image registration by camera 1. 136 Results obtained by the experimenters are indicated with the subscripts  $_{VS1}$ 137 and  $_{VS2}$  (visual, simultaneous). In addition, a second camera (Camera 2; 138 Samsung Galaxy S5, Model No.: SM-G800F, OS: Android 4.4.2) was used to 139 collect simultaneous close-up images of the sludge blanket at time intervals 140 of 30s by means of frame lapse recording software (Framelapse by Neximo 141 Labs, v2.1.1). Camera 2 was moved manually during each batch experiment 142 by a third experimenter so to match the visually recognized SBH as close as 143 possible. Results obtained with the close-up images are referred to by the 144 subscript  $_{\rm VO}$  (visual, off-line). 145

# 146 2.2. Shape Constrained Spline Function Fitting

The proposed image-based sludge blanket registration method consists of 147 an extension of the pre-existing SCS method reported in Villez et al. (2013). 148 Whereas the original method only allows analysis of univariate signals, the 149 extended method permits simultaneous fitting of multiple SCS functions to 150 multivariate data series. Each of fitted functions is however subject to the 151 same shape constraints. Each part of the method SCS method is introduced 152 generally followed by a discussion of details pertaining to the analysis of 153 image data. 154

# 155 2.2.1. Modeled Data

General treatment. The measurements are given as a  $J \times K$  matrix  $\tilde{Y}$ of which  $y_{j,k}$  is the element in the *j*th row and *k*th column and  $\tilde{Y}_{.,k}$  is the *k*th column vector. Each row vector  $\tilde{Y}_{j,.}$  is associated with the *j*th element of  $\boldsymbol{x}$  which is the  $J \times 1$  vector containing the values of a single independent 160 variable.

Application. The analyzed data sets correspond to rectangular selections 161 of red-blue-green images (see the Supplementary Information, Fig. S.1). A 162 rectangular section of the image is selected so that the horizontal dimension 163 of the selection covers the center of the photographed column and has the 200 164 mL and 1000 mL marks on the column as limits in the vertical dimension. 165 The width of the section is arbitrarily set to 51 pixels for all experiments. 166 The heights of the image sections changed slightly across experiments and 167 are reported in Table 1. All color channels (3) are included for analysis. 168

The data in each image are initially organized as a 3-D array with dimen-169 sions corresponding to the vertical image dimension, the horizontal image 170 dimension, and the color channel. For the purpose of analysis, we consider 171 each set of 51 light intensities corresponding to the same vertical position 172 and color channel as repeated measurements of the same light intensity. To 173 generate a 2-D matrix of the form  $\tilde{Y}$  the following unfolding procedure is 174 executed. One first retrieves the matrix of light intensity values in the top 175 row of pixels in the image and defines this matrix as Y. This matrix has 176 dimensions  $51 \times 3$ . One continues by selecting the same matrix for the sec-177 ond row and places this matrix below the previously obtained matrix. This 178 concatenation process is continued until the bottom row pixels are reached 179 and added. At this stage, the matrix  $\hat{Y}$  is completed. The corresponding 180 vector  $\boldsymbol{x}$  contains the row pixel index for each row in  $\tilde{\boldsymbol{Y}}$ . In the case of ex-181 periment 6, the dimensions of the matrix  $\tilde{Y}$  are  $J = 1287 \times 51 = 65637$  and 182 K = 3. The independent data vector ( $\boldsymbol{x}$ ) contains the corresponding pixel 183 positions, meaning that each of the 1287 vertical pixel positions appears 51 184

185 times within x.

# 186 2.2.2. Data Model and Definition of Optimality

*General treatment*. The multivariate data series are modeled by means of 187 K spline functions,  $f_k(\boldsymbol{\beta}, \boldsymbol{x})$  (k = 1, ..., K) (Ramsay and Silverman, 2005). 188 The choice for spline functions is especially motivated by the fact that shape 189 constraints applied to non-empty intervals of a spline function domain can 190 be formulated as a finite number of equality and inequality constraints (see 191 e.g., Papp and Alizadeh, 2014; Villez et al., 2013; Villez and Habermacher, 192 2016). The degrees of the spline functions are given as  $D_k$ . Internal spline 193 knots determine where one polynomial segment ends and the next one starts. 194 They can be placed in arbitrary locations within  $[x_1, x_J]$ . Because of our 195 function choice, each function is linear in the spline coefficients (function 196 parameters). More specifically, the spline function model generates estimates 197 of the measured variables  $(\mathbf{Y})$  given function parameters  $(\boldsymbol{\beta})$  as follows: 198

$$\boldsymbol{Y}(\boldsymbol{\beta}) = \boldsymbol{f}(\boldsymbol{\beta}, \boldsymbol{x}) \tag{1}$$

199 with:

$$\boldsymbol{f}(\boldsymbol{\beta}, \boldsymbol{x}) = \begin{bmatrix} f_1(\boldsymbol{\beta}_1, \boldsymbol{x}) & \dots & f_k(\boldsymbol{\beta}_k, \boldsymbol{x}) & \dots & f_K(\boldsymbol{\beta}_K, \boldsymbol{x}) \end{bmatrix}$$
$$= \begin{bmatrix} \boldsymbol{B}_1(\boldsymbol{x}) \ \boldsymbol{\beta}_1 & \dots & \boldsymbol{B}_k(\boldsymbol{x}) \ \boldsymbol{\beta}_k & \dots & \boldsymbol{B}_K(\boldsymbol{x}) \ \boldsymbol{\beta}_K \end{bmatrix}$$
(2)

$$\boldsymbol{\beta} = \left[ \boldsymbol{\beta}_1^{\mathrm{T}} \quad \boldsymbol{\beta}_2^{\mathrm{T}} \quad \cdots \quad \boldsymbol{\beta}_k^{\mathrm{T}} \quad \cdots \quad \boldsymbol{\beta}_K^{\mathrm{T}} \right]^{\mathrm{I}}$$
(3)

In the above, the matrices  $B_k(x)$  correspond to the evaluation of the spline basis of the kth function in the arguments x. The model is fitted to the data by minimizing the following least-squares lack-of-fit:

$$g(\boldsymbol{\beta}) = \sum_{j=1}^{J} \sum_{k=1}^{K} \left( \tilde{\boldsymbol{Y}}_{j,k} - \boldsymbol{Y}_{j,k}(\boldsymbol{\beta}) \right)^2$$
(4)

For primers on spline models, we refer to Hastie et al. (2001) and Ramsay and Silverman (2005).

Application. In the present study, three natural cubic (K = 3) B-spline 206 functions are fitted to three column vectors of  $\boldsymbol{Y}$ . Internal spline knots are 207 placed at every 8th pixel following the first pixel for all functions (i.e.,  $x_9$ , 208  $x_{17},\ldots$ ). This knot placement was found to deliver sufficient flexibility to 209 the fitted functions while ensuring a reasonably short computational effort. 210 As both the knot locations and independent data vectors are the same for 211 each function, the matrices  $\boldsymbol{B}_k(\boldsymbol{x})$  are the same for every function (i.e.,  $\boldsymbol{B} =$ 212  $\boldsymbol{B}(\boldsymbol{x}) = \boldsymbol{B}_k(\boldsymbol{x}), k = 1, \dots, K).$ 213

#### 214 2.2.3. Shape Constraints

General treatment. During model fitting, the spline functions are con-215 strained to have a predefined shape. The assumed shape can be derived from 216 expert knowledge or based on rigorous qualitative simulation (Kuipers, 1994; 217 Shaich et al., 2001; Bredeweg et al., 2009). In either case, the shape is defined 218 as a sequence of E episodes  $(e = 1, \ldots, E)$ . These episodes are contiguous 219 intervals of the function domain within which a number of the function's 220 derivatives do not change sign. Such a sequence is known as a *qualitative se*-221 quence. It is defined mathematically as a matrix  $\boldsymbol{S}$  with  $\boldsymbol{S}(e, d+1) = s_{e,d+1}$ 222 specifying the sign of the dth derivative in the eth episode. The elements of S223

can taken on the integer values +1, 0, and -1 to indicate positive, zero, and negative signs of the derivatives. When the sign is unspecified, a question mark (?) is used instead. The matrix  $\boldsymbol{S}$  is specified a priori. The episodes themselves are defined by T = E - 1 transitions,  $\boldsymbol{\theta}$  ( $\theta_t = \boldsymbol{\theta}(t)$ ; t = 1, ..., T), which are the function argument values where the episodes meet and which need to be estimated. The complete description of the shape of a function by means of  $\boldsymbol{S}$  and  $\boldsymbol{\theta}$  is known as a qualitative representation (QR).

Application. The fitted functions are constrained to have a shape defined by two episodes. The first episode has a concave shape, i.e. a negative sign for the second derivative. The second episode has a convex shape and decreasing. Consequentially, one writes  $\boldsymbol{S}$  as a matrix with two rows, one for each episode:

$$\boldsymbol{S} = \begin{bmatrix} ? & ? & -1 & ? \\ ? & -1 & +1 & ? \end{bmatrix}.$$
 (5)

The corresponding QR thus exhibits a single transition which corresponds to the location of the inflection point between the two episodes:  $\boldsymbol{\theta} = \boldsymbol{\theta} = \boldsymbol{\theta}_1$ .

# 233 2.2.4. Optimization

*General treatment.* With the above definitions, the least-squares SCS function fitting problem is written mathematically as follows:

$$\hat{\boldsymbol{\beta}}, \hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\beta}, \boldsymbol{\theta}} g(\boldsymbol{\beta}, \boldsymbol{\theta}) = \sum_{j=1}^{J} \sum_{k=1}^{K} \left( |\boldsymbol{Y}_{j,k} - \boldsymbol{Y}(\boldsymbol{\beta})_{j,k}|^2 \right)$$
(6)

s.t. 
$$\boldsymbol{\beta} \in \Omega(\boldsymbol{\theta}, \boldsymbol{S})$$
 (7)

$$\boldsymbol{\theta} \in \Theta \tag{8}$$

and subject to the linear constraints Eq. 1–3. In the above,  $\Theta$  is the set containing all feasible values for  $\boldsymbol{\theta}$  and  $\Omega(\boldsymbol{\theta}, \boldsymbol{S})$  is the set containing all values for  $\boldsymbol{\beta}$  satisfying the shape constraints.  $\Theta$  is defined mathematically as follows:

with  $f_k^{(d)}(\cdot, u)$  the *d*th derivative of  $f_k(\cdot, u)$  with respect to u.

The objective function (Eq. 7) is quadratic in  $\beta$ . The shape constraints (Eq. 9) are convex in  $\beta$ . In the case of univariate spline functions, as in this study, they can be formulated as a finite number of necessary and sufficient inequality constraints (Papp and Alizadeh, 2014). As a result, the problem has a single optimum and can be solved efficiently to global optimality given values for  $\theta$ . Consequentially, the complete optimization problem can be solved as a nested optimization problem where the values for  $\beta$  are repeat-

edly obtained for considered candidate values for  $\boldsymbol{\theta}$ . The above problem is 248 however non-convex and possibly multi-modal in  $\boldsymbol{\theta}$ . Still, globally optimal 249 estimates for  $\boldsymbol{\theta}$  can be found by means of the branch-and-bound algorithm as 250 used in Villez et al. (2013); Villez and Habermacher (2016). The bounding 251 procedures and their proofs are similar to those presented in Villez et al. 252 (2013); Villez and Habermacher (2016) and are given in the Supplementary 253 Information. Importantly, the bounding gap does not converge to zero in 254 the multivariate case, in contrast to results obtained for the univariate case 255 (K = 1) studied in Villez et al. (2013). This situation is however similar to 256 the case studied in Villez and Habermacher (2016), where the presence of 257 discontinuous trends in univariate data series was explicitly accounted for. 258 For more details we refer to the Supplementary Information. 259

Application. The feasible set for the transition is the function domain, i.e.  $\Theta := [x_1, x_J]$ . Optimization of  $\boldsymbol{\theta}$  is continued until a tolerance of 1/8 of a pixel is achieved for the optimal position of the inflection point. This optimization is repeated for each image registered with camera 1 in each of the experiments. For a given experiment, the obtained value ( $\hat{\theta}$ ) for image *i* is given as  $\hat{\theta}_{SCS,i}$ .

# 266 2.3. Sludge Blanket Height Registration Methods

SBH estimates are obtained with four distinct methods. The first two methods are automated. A third method is based on off-line visual inspection of the close-up images of the sludge blanket. The fourth method consists of registering the SBH visually during the batch experiments by two experienced experimenters. More details follow next.

# 272 2.3.1. Automated Sludge Blanket Height Registration with the Shape Con 273 strained Splines Method

Following optimization as described above, the location of the inflection points ( $\theta$ ) are given as a vertical pixel position (direction: top-down) within the analyzed segment of the images. To obtain the SBH for image *i* in a given experiment, measured from the bottom of the glass column, the following linear expression is used:

$$\hat{h}_{\text{SCS},i} = h_L + (h_U - h_L) \cdot \left(1 - \frac{\hat{\theta}_{\text{SCS},i} - x_J}{x_1 - x_H}\right), \quad i = 1, \dots, I$$
 (10)

with previously undefined parameters given in Table 1. The complete time series of SBH estimates is given as the vector  $\hat{h}_{SCS}$  and the corresponding sampling time vector as  $\boldsymbol{z}_{SCS}$ .

# 282 2.3.2. Automated Sludge Blanket Height Registration with the Maximum Slope 283 Method

In Kim et al. (2011) an image analysis method for sludge blanket registration is proposed and positively evaluated. For every pixel along the vertical column dimension, one computes a slope parameter,  $S_j$ , as the difference between the light intensity at the considered pixel and the light intensity at the lowest pixel divided by the absolute distance between the considered pixel and the lowest pixel:

$$S_j = \frac{y_j - y_J}{|x_j - x_J|}$$
(11)

with  $y_j$  and  $y_J$  light intensities for a single color channel obtained within 290 a single column of pixels. The pixel j corresponding to a maximal slope 291 is referred to as the knee in the light intensity profile and is identified as 292 the sludge blanket height. Note that the definition of such a knee is different 293 from the definition of an inflection point. In Kim et al. (2011) this is executed 294 with only one column of pixels in the recorded images and with the red color 295 channel only. Following pixel location, the sludge blanket height is computed 296 by linear interpolation as above ((10)). The maximum slope (MS) method is 297 implemented as in Kim et al. (2011) except for the following modifications: 298

Instead of selecting one column of pixels, the light intensity data are
 averaged along the horizontal dimension prior to analysis. The pixel
 selection is the same as for the shape constrained spline method.

20. Instead of computing the slope for every pixel, the slope is only computed for the first 1250 pixels. This avoids errors due to noise as will
be demonstrated below.

The sludge blanket heights obtained with the MS method are reported as  $\hat{h}_{MS}$  and the corresponding time instants as  $\boldsymbol{z}_{MS}$ .

# 2.3.3. Visual Sludge Blanket Height Registration via Close-up Inspection af ter Experimentation

The third method to establish SBH estimates is based on a visual inspection of close-up images after the experiment is finished. The close-up images are used as a reference in what follows. The obtained SBHs are given as the vector  $\hat{h}_{VO}$ . The corresponding time instants are given as  $\boldsymbol{z}_{VO}$ .

# 2.3.4. Conventional Sludge Blanket Height Registration during Experimenta tion

A 4th and 5th SBH estimate is obtained by means of a visual inspection of the glass column during the batch experiment. These SBH estimates are referred to as  $\hat{h}_{VS1}$  and  $\hat{h}_{VS2}$ . The times of registration are the same for both estimates and are given as  $\boldsymbol{z}_{VS}$ .

# 319 2.4. Zone Settling Velocity Estimation

Each of the obtained SBH profiles can be used to model hindered and 320 compressed settling in detail as described in Torfs et al. (2016) and as also dis-321 cussed in the introduction. Given our focus on SBH registration, we demon-322 strate the utility of the method by computing the ZSV, which reflects on the 323 hindered settling only and is conceptually simpler compared to compressed 324 settling model identification procedures. The ZSV is computed by means of 325 locating the inflection point with negative tangent slope in the considered 326 SBH profile (e.g., Vanderhasselt and Vanrolleghem, 2000). Indeed, the shape 327 of the profile is known to consist of a downward concave episode followed by 328 a downward convex episode with the transition corresponding to the SBH. 329 The sign matrix  $\boldsymbol{S}$  thus is: 330

$$\boldsymbol{S} = \begin{bmatrix} ? & - & - & ? \\ ? & - & + & ? \end{bmatrix}$$
(12)

To obtain the ZSV from the SBH estimates obtained via SCS-based image analysis, the optimization problem described above (Eq. 7–9) is modified as follows. The data model is changed so that the univariate vector containing the SBH profile are approximated with a single univariate cubic splinefunction with knots at every sampling time:

$$K = 1 \tag{13}$$

$$\tilde{\boldsymbol{Y}} = \tilde{\boldsymbol{Y}}_{\cdot,1} = \tilde{\boldsymbol{y}}_k = \hat{\boldsymbol{h}}_{\text{SCS}}$$
(14)

$$\boldsymbol{x} = \boldsymbol{z}_{\text{SCS}} \tag{15}$$

All other settings are kept the same so that a least-squares fit of a SCS 336 function to the SBH profile is obtained. Importantly, the modified optimiza-337 tion problem reduces to the univariate case studied in Villez et al. (2013). 338 As a result, the best location of the inflection point can be determined with 339 absolute precision and global optimality. Upon fitting the SCS function, the 340 ZSV is obtained by computing the first derivative (tangent slope) in the in-341 flection point. The absolute tangent slope is reported as the ZSV. This is 342 executed for every experiment. 343

The above computation of the ZSV is also executed for the SBH estimates obtained with off-line and simultaneous visual inspection by replacing the dependent data vector  $\tilde{\boldsymbol{y}}_k$  with the data series containing the SBH estimates ( $\hat{\boldsymbol{h}}_{\text{VO}}$ ,  $\hat{\boldsymbol{h}}_{\text{VS1}}$ ,  $\hat{\boldsymbol{h}}_{\text{VS2}}$ ,  $\hat{\boldsymbol{h}}_{\text{MS}}$ ) and the independent data vector with the corresponding image and SBH registration times. The ZSVs are obtained for experiments 5 and 6.

### 350 2.5. Data and Software

All data and software required to reproduce the results of this study are released publicly with a GPL v3 license and are added to the *Supplementary Information*.

# 354 3. Results

# 355 3.1. Demonstration of the Shape Constrained Splines Method for Automated 356 Sludge Blanket Height Registration

Fig. S.1 shows a section of a single image obtained during experiment 5. 357 The pixels selected for further analysis are indicated with yellow lines. Fig. 2 358 shows the corresponding light intensity measurement as a function of the 359 pixel index for the three channels. While the data series exhibit considerable 360 levels of noise, one clearly observes the sludge blanket as an inflection point 361 in the data series. The inflection point corresponds to the discontinuity in the 362 sludge concentration better known as the SBH. Solving the SBH estimation 363 problem (Eq. 7–9) delivers three optimized SCS functions -one for each color 364 channel- with the same concave-convex shape and the same location for the 365 inflection point. The SCS functions and the pixel index corresponding to the 366 identified sludge blanket (1056) are also shown in Fig. 2. 367

# 368 3.2. Demonstration of the Maximum Slope Method for Automated Sludge Blanket Height Registration

In the top panel of Fig. 3 one can see the average light intensity for the 370 red color channel as a function of the pixel index for image considered above. 371 The slope values are given in the bottom panel. One can see that selecting 372 the pixel with the MS method results in the selection of the second last pixel 373 at the bottom the image. This is caused by substantial noise amplification of 374 the slope computation especially close to the reference pixel at the bottom 375 of the image. The modified method considering the top 1225 pixels selects 376 pixel 977, which is a more sensible choice. However, a human observer may 377

instead select pixel 1035 as the knee. This difference is again explained by noise amplification of the slope computation. However, even pixel 1035 is higher in the image compared to the shape constrained spline method result (1056). This is explained by the fact that the maximal slope method selects a location for a knee point rather than an inflection point.

# 383 3.3. Sludge Blanket Height Profiles

Fig. 4 shows a composite image obtained by collating the analyzed seg-384 ments of the images taken from the 127 consecutive images collected dur-385 ing experiment 5. The image is presented here without any modification, 386 mainly to visualize the rather low contrast in the collected images. The pixel 387 heights corresponding to the SCS-based inflection points ( $\theta_{SCS}$ ) and the MS 388 knee  $(\hat{\boldsymbol{\theta}}_{MS})$  are also indicated in the collated image. Close inspection reveals 389 that the SCS-based inflection points correspond to the SBH at the front of 390 the cylindrical column. One can see a semi-dark area above the identified 391 inflection points. The top of the semi-dark area correspond to the back of 392 the cylindrical column. The fact that the front and back side of the sludge 393 blanket can be distinguished is a consequence of the applied position and 394 angle of the camera. The MS knee pixel cannot be tied easily to any of the 395 two sludge blanket features in the images. In addition, the MS knee profile 396 appears to be more erratic than the profile of the inflection points. The col-397 lated images with and without SBH estimates obtained for all experiments 398 are available in the Supplementary Information. 399

In experiments 5 and 6, all considered methods for SBH registration were applied. In Fig. 5 one can see the obtained SBH estimates. The SBH estimates obtained with close-up visual inspection and by simultaneous visual inspection ( $\hat{h}_{VO}$ ,  $\hat{h}_{VS1}$ , and  $\hat{h}_{VS2}$ ) appear fairly close to each other. The SCSbased SBH estimates ( $\hat{h}_{SCS}$ ) are about 70 mL higher in the concave episode (hindered and compressed settling) for experiment 5 and about 30 mL lower for experiment 6. For the MS method, the offset is +100 mL for experiment 5 and -5 mL for experiment 6.

Each of the obtained SBH profiles shown in Fig. 4 and Fig. 5 can be de-408 scribed as a decreasing trend that is composed of a concave episode followed 409 by a convex episode. As in previous studies (e.g., Diehl, 2015), the concave 410 episode is explained as a result from turbulence stemming from the stirring 411 and possibly flocculation before the start of the experiment. Such behavior 412 is generally considered non-ideal as the first data points do not provide in-413 formation about the settling process. To account for this, one can model the 414 effect of turbulence explicitly (e.g., Diehl, 2015) or manipulate the data to 415 remove the concave episode entirely (e.g., De Clercq, 2006). In this work, we 416 fit a shape constrained spline function to the SBH profiles with the desired 417 concave-convex shape. The resulting functions for experiments 5 and 6 are 418 shown in Fig. 5. The standard error for each SBH measurement profiles, 419 obtained by taking the fitted curve with the close-up SBH profile  $(h_{\rm VO})$  as 420 a reference, are reported in Table 2. The reference curve fits the close-up 421 SBH profile best, as expected since  $h_{\rm VO}$  were used to fit the reference curve. 422 The worst standard error is obtained by the MS method in both experiments 423  $(h_{\rm MS})$ . The best standard error, apart from the result with close-up data, 424 is obtained with the data produced by one human experimenter, which is 425 however different in each experiment  $(\mathbf{h}_{VS1}, \mathbf{h}_{VS2})$ . In each experiment, the 426 SCS-based SBH data  $(\hat{h}_{SCS})$  leads to a standard error that is smaller than 427

<sup>428</sup> one of the standard errors obtained by the human experimenters.

The curve-fitting is also executed for the other experiments by using the 429 SBH profiles obtained the MS and SCS methods. Table 3 lists the obtained 430 coefficients of determination  $(R^2)$ . One can see that  $R^2$  is above 0.995 in all 431 cases except for the MS method, which delivers  $R^2$  values as low as 0.235. 432 This means that the SBH measurement profiles satisfy the expected concave-433 convex shape very well, except for the profiles obtained with the MS method. 434 The corresponding SBH profiles  $(\hat{h}_{MS})$  and the fitted curves are displayed in 435 the Supplementary Information. Visual inspection allows to conclude that 436 the MS method remains extremely sensitive to noise. Indeed, the MS method 437 frequently identifies pixels that are close to the bottom of the image due 438 to the high noise in the computed slopes. Several tests were executed to 439 evaluate whether the considered set of pixels could be expanded or reduced 440 (above/below 1225 pixels). However, in the 8th and 9th experiment the 441 sludge blanket at the end of the experiment is located close to the 1225th 442 pixel so that further decreases are difficult to motivate. At the same time, 443 the results for experiment 1 show sensitivity to noise at the start of the 444 experiment. Expanding the considered pixel selection makes things even 445 worse. It is therefore impossible to define a single set of top-most pixels 446 to be considered in the MS method in such a way that low sludge blanket 447 levels can be identified while also avoiding errors due to noise amplification 448 for pixels close to reference pixel at the bottom of the images. Given such 449 poor performance, further analysis excludes results on the basis of the MS 450 method. 451

### 452 3.4. Zone Settling Velocity Estimation

As indicated above, computing the ZSV is one way to usefully interpret 453 the obtained SBH profiles. The curve fitting described above identifies the 454 location of the inflection point at the concave-convex intersection of the SBH 455 profile. As is typically assumed, the ZSV corresponds to the slope of the 456 tangent in the inflection point located at the transition from the concave 457 to the convex episode. In experiment 1 to 8, the obtained tangent lines 458 appear sensible based on visual inspection (see Fig. 5 and the Supplementary 459 Information. For experiment 9 the time needed for the transition from the 460 zone settling phase to the compressed settling phase is extremely short which 461 likely affects the accuracy of the estimated slope of the tangent line, as also 462 discussed in van Loosdrecht et al. (2016). 463

All slopes of the identified tangent lines correspond to settling velocities 464 and are shown in the top panel of Fig. 6. As expected, the obtained settling 465 velocities follow a decreasing concave trend. In addition, the results obtained 466 with visual estimates are generally consistent with the SCS-based results 467 (maximum 27% relative difference). A conclusive validation would however 468 require additional samples. A fit of the Vesilind equation  $(v(c) = v_0 e^{-r_v c})$ , 469 with c the sludge concentration, v(c) the ZSV, and  $v_0$  and  $r_v$  parameters) is 470 shown as well and delivers an R2 value of 0.95. As an alternative, a fit of a 471 rational equation (Eq. 28, Diehl, 2015) is also shown. This rational equation 472 has three parameters and delivers an  $R_2$  value of 0.86. Both equations thus 473 fit the data well and cannot not be discriminated easily. The bottom panel 474 shows the corresponding settling flux  $(q(c) = v(c) \cdot c)$  which is typically used 475 for the determination of the settling capacity of secondary settlers. Note 476

that the Vesilind and rational equations are designed to describe the settling
behavior at relatively high concentrations where zone settling occurs. It is
therefore not surprising that the curves have a different shape in the low
concentration region.

# 481 4. Discussion

#### 482 4.1. Main Results and Major Benefits of the Proposed Method

Image analysis was executed for the first time by means of a method for qualitative trend analysis, particularly on the basis of an SCS model. Furthermore, automated SBH registration is benchmarked for the first time against a pre-existing image analysis method for SBH registration and conventional SBH registration by human experimenters. Based on our results, several benefits of the proposed method when applied for image analysis during batch settling experiments have been demonstrated:

The images were obtained with an off-the-shelf digital camera, all code
is released publicly, and both experiments and image analysis can be
executed in a standard laboratory environment. Consequentially, the
method is accessible to many in the field, in contrast to alternatives
which rely on equipment and software that is expensive to obtain and
maintain.

The SCS data model allows automatic SBH estimation based on light
 intensity profiles extracted from digital images recorded during batch
 settling experiments. As demonstrated, this is also possible despite the
 collection of rather noisy images. In contrast, the pre-existing maxi mum slope (MS) method is very sensitive to noise. Because of this,

we expect our method to fare well even in cases where the supernatant remains turbid, e.g. when pin-point flocs are present.

• The SCS data model fits curves to the complete light intensity profiles and all color channels at once. Put otherwise, *(i)* all available information is incorporated in the image analysis, *(ii)* noise amplification due to differentiation is avoided, and *(iii)* information removal and biasing effects of data filtering are absent.

The combined experimental and data-analytic method prevents human 508 error and subjective analysis by automating the SBH registration via 509 deterministic optimization. In contrast, conventional approaches may 510 suffer from uncertainty stemming from subjectivity of human experi-511 menters as well as variability of the exact method. Such variability may 512 stem from the application of different practices in different regions, in 513 individual wastewater treatment plants, by individual operators, and 514 over time. 515

In its current form, our image-based analysis is considered attractive to 516 academic experimenters primarily as a way to increase the efficiency of ex-517 perimental data collection, possibly enabling the execution of measurement 518 campaigns over long periods or with a high measurement frequency. It may 519 also be useful in full-scale activated sludge WWTPs where an early-stage 520 warning of deteriorating sludge settling properties is warranted. Importantly, 521 routine application requires as much sample preparation as is necessary to 522 obtain the diluted sludge settling index (DSVI) given that the time spent on 523 sludge blanket registration with the human eye can be omitted. 524

At the same time, our results lead to acceptable but still considerable devi-525 ations between the results obtained with the SCS-method and those obtained 526 with human-eye based SBH profiles. The number of experiments executed to 527 develop and demonstrate the SCS-method are however too low to establish 528 whether the observed deviations are of a systematic or random nature. In 529 addition, it is unclear whether the larger errors should be expected in the 530 human-eye SBH profiles or the SCS-based profiles. Our initial experiences 531 suggest that human-eye SBH profiles can exhibit some lag during the time 532 zone-settling dominates, especially when the sludge blanket is not defined 533 well yet. Indeed, the fast-forming and fast-moving sludge blanket can be 534 hard to track in time by the human eye. Regardless of such differences, the 535 SCS-based method also offers the ability to obtain an objective SBH reading 536 rather than a reading prone to human error and subjectivity. 537

#### 538 4.2. Expanded Range of Qualitative Trend Analysis Applications

Historically speaking, qualitative trend analysis methods, including the 539 original SCS method, were proposed to tackle extrapolation issues in fault 540 diagnosis (see e.g. Maurya et al., 2007; Villez et al., 2013). Recent work 541 expanded the range of applicability of such methods to fault detection in 542 sequencing batch reactors (Villez and Habermacher, 2016), ammonia control 543 (Thürlimann et al., 2015) and dynamic model identification (Mašić et al., 544 2017). SCS-based data modeling is especially valuable when models which 545 are entirely mechanistic in nature are prohibitively expensive to obtain. The 546 current study expands the application range of the SCS data model further 547 into the field of image analysis and characterization of separation processes. 548 Thus, our current results further demonstrate the general applicability of 549

<sup>550</sup> qualitative trend analysis methods and SCS-based methods in particular.

# 551 4.3. Perspectives

Given the promising results in this study, several new questions can be raised. The following topics are of primary interest:

- 1. Is the image analysis method robust enough to handle several sludge
  types without further modification?
- 2. Can the image analysis method also be used for experimentation with
  highly diluted sludges whose settling is of Stokesian nature?
- 3. Are the obtained SBH profiles useful for more complex modeling tasks
  such as the joint modeling of hindered and compressed settling? This
  may be the case but it is unclear yet whether the SCS-based SBH
  profiles are of sufficient quality.
- 4. Can the time savings obtained by avoiding human-eye sludge blan-562 ket reading be increased further by enabling the execution of multiple 563 simultaneous settling experiments and/or by providing a sludge sam-564 ple preparation device that does not modify the flocculation state? If 565 possible, the SBH registration method combined with automated sam-566 ple preparation will finally enable the evaluation of predictive control 567 strategies based on solid flux theory, including automated control of 568 the recycle flow rate, step feed flow rate, step sludge flow rates, and 569 temporary sedimention in aeration tanks. 570
- <sup>571</sup> Based on current experience the authors are convinced that the answer to <sup>572</sup> each of the above questions is yes. However, further experimental evidence is

warranted. In any case, our experiments suggest that the desired experimental evidence can now be collected in an objective and time-efficient manner.

#### 575 5. Conclusions

Automatic registration of the sludge blanket height in settling experi-576 ments is demonstrated to be feasible via image analysis. The image analysis 577 procedure is based on a multivariate extension of the shape constrained spline 578 method. Promising results were obtained with inexpensive equipment acces-579 sible to any laboratory. It is especially noteworthy that the shape constrained 580 splines method appears fairly robust against large levels of noise and the ob-581 tained results compare fairly to conventional sludge blanket height registra-582 tion methods. Most importantly, we consider our study the first step towards 583 a fully automated, reliable, and economical alternative to existing methods 584 for sludge blanket height registration. 585

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Table 1: List of batch settling experiments. Experiments marked with <sup>(\*)</sup> are those experiments for which visual registration of the sludge blanket height was performed by two human experimenters (during the experiment) and by visual inspection of close-up images (after the experiment).

Experiment index	Original sludge sample	Concentration	Pixel height
		m g/L	J
1	1	2.40 (no dilution)	1275
2	1	1.92	1282
3	1	1.54	1285
4	1	1.22	1285
$5^{(*)}$	2	1.20	1286
6 (*)	2	1.00	1287
7	2	0.86	1289
8	2	0.74	1279
9	2	0.58	1287

Table 2: Standard error (in mL) obtained by considered the deviations between the SBH measurements and the curve fitted to the SBH measurement obtained by close-up image inspection (VO).

Experiment index	Method				
	SCS	MS	VO	VS1	VS2
5	18.3	37.9	2.51	7.37	32.6
6	23.9	36.3	5.19	41.1	21.5

Experiment index	Method				
	SCS	MS	VO	VS1	VS2
1	0.9999	0.5607			
2	0.9999	0.9972			
3	0.9999	0.8036			
4	0.9997	0.8795			
5	0.9998	0.9972	1.0000	1.0000	0.9975
6	0.9990	0.9989	0.9994	0.9998	1.0000
7	0.9993	0.8027			
8	0.9990	0.8580			
9	0.9954	0.2353			

Table 3: Coefficients of determination  $(R^2)$  for the curves fitted to each of the sludge blanket height profiles.



Figure 1: Scheme of the experimental setup. Camera 1 is positioned level to the top surface of the sludge sample. Camera 2 is adjusted manually during each experiment to take close-up images of the sludge blanket. Human inspection is executed in such a way that the lines of sight of the cameras are not interrupted.



Figure 2: Experiment 5 - Image 42. Dots: Light intensity data; Dashed white lines: Fitted shape-constrained spline functions; Full black vertical lines: Identified inflection point location. The shape constrained splines method located the inflection point in the light intensity data successfully and is consistent with a visual assessment of the sludge blanket height.



Figure 3: Experiment 5 - Image 42. (Top) Dots: Averaged red channel light intensity data; Dotted vertical line: Pixel location obtained with maximal slope method considering every pixel; Dashed vertical line: Pixel location obtained with maximal slope method considering only the first 1225 pixels; Full vertical line: Pixel location obtained via shape-constrained spline function fitting; Circles and connecting full line: vizualization of the maximal slope when considering only the first 1225 pixels. (Bottom) Dots: Computed slopes; Dotted vertical line: Pixel location obtained with maximal slope method considering every pixel; Dashed vertical line: Pixel location obtained with maximal slope method considering only the first 1225 pixels; Full vertical line: Pixel location obtained via shape-constrained spline function fitting; Circles and horizontal full line: vizualization of the maximal slope when considering only the first 1225 pixels. The maximum slope method delivers results that are fairly different from the result obtained with the shape constrained splines method.



Figure 4: Experiment 5. Composite image showing data from 127 consecutive images. Green arrows are used to indicate the sludge blanket at the front and back of the column recognized by close visual inspection. Yellow cross-hairs indicate the sludge blanket height estimates obtained by means of the shape constrained splines method and correspond to the front of the column. Red cross-hairs indicate the sludge blanket height estimates obtained by means of the maximum slope method. The red cross-hairs do not match any obvious feature in the image and follow an irregular pattern.



Figure 5: Registered batch settling curves: *Top*: Experiment 5; *Bottom*: Experiment 6. SCS-based sludge blanket height profiles (green dots,  $\hat{h}_{SCS}$ ), MS-based sludge blanket height profiles (blue dots,  $\hat{h}_{MS}$ ) and profiles based on visual registration (red, yellow, and purple dots;  $\hat{h}_{VO}$ ,  $\hat{h}_{VS1}$ , and  $\hat{h}_{VS2}$ ). A spline function with a concave-convex shape (full grey line) is fitted to the  $\hat{h}_{SCS}$  data (SBH data - SCS). The tangent line in the inflection point of the shape constrained splines function is shown with a dashed black line. The modeling errors (grey circles) show that the curve fits the data well in both experiments.



Figure 6: Use of the ZSV to characterize dynamic sludge settling properties. *Top:* Zone settling velocity (ZSV) as a function of the sludge concentration. All ZSVs are shown together with a least-squares fit of the Vesilind and Diehl equations. The experiment number is added at the top of the image right above the corresponding solids concentration. *Bottom:* Settling flux curve obtained based on the fitted Vesilind and Diehl equations.

### 732 S. Supplementary Information

The Supplementary Information includes additional details regarding the experimental method (Section S.1), the SCS modeling method (Section S.2), additional figures (Section S.3), and all data and software to reproduce our results (separate .zip file).

#### 737 S.1. Experimental protocol

The following description of a single experiment is added to ensure broad applicability of the SCS-based SBH registration method.

- 740 S.1.1. Hardware and consumables
- <sup>741</sup> Prior to the experiment, collect and prepare the following materials:
- A 2 L clear glass cylinder with coloured tape added to mark the 200
  mL and 1000 mL levels. Take note of the distance between these two
  levels.
- <sup>745</sup> 2. A white panel to place behind the 2 L cylinder.
- 3. An off-the-shelf digital camera, equipped with a continuous power supply and programmed to continuously collect an image at a fixed time
  interval.
- 4. A diluted sludge sample of at least 2 L with known solids concentration.
  5. A stirring rod
- 751 S.1.2. Protocol
- <sup>752</sup> Execute the following steps in the laboratory:
- 1. Place the camera, cylinder, and panel on a single line on a horizontalplatform.

- Position the camera so that the line-of-sight corresponds to a horizontal
  line aligned with the 2000 mL mark on the cylinder.
- a. ensure that the positions of the camera, cylinder, and panel do not
  change during the experiment.
- 4. Start the image collection program on the camera.
- 5. Fill the cylinder with the 2 L of the diluted sludge sample.
- 6. Stir the sample with the stirring rod.
- 762 7. Stop stirring right before the recording of an image and record the time763 stirring was halted.
- 8. Let the sludge settle for as long as considered necessary (e.g., 30 minutes).
- 9. Stop the image collection program on the camera.
- <sup>767</sup> 10. Empty and clean the cylinder.
- The following steps are executed after the experiment is executed.
- <sup>769</sup> 1. Collect all images from the camera.
- 2. Select all images of interest starting with the image where stirring wasstopped first.
- 3. Select a section in the images corresponding to the center of the cylinder
  and covering the 200 mL to 2000 mL range of the column.
- 4. Apply the SCS method to find the pixel corresponding to the sludgeblanket in an image section. Apply this to every image section.
- 5. Convert the sludge blanket pixels to a sludge blanket height (SBHs) bylinear interpolation.

# 778 S.2. Description and proofs of applied bounding procedures

In the next paragraphs, the necessary elements contributing to the globally optimal solution of the SCS optimization problem discussed in the text are explained in detail. Additional symbols not used in the main text are given in Table S.1.

Symbol	Definition
$oldsymbol{eta}^{ ext{L}}$	Lower bound values for of all spline function coefficients
$oldsymbol{eta}^{\mathrm{U}}$	Upper bound values for of all spline function coefficients
$\epsilon$	Bounding gap tolerance
$\underline{\theta_t}$	Lower bound for $\theta_t$
$\overline{ heta_t}$	Upper bound for $\theta_t$
$oldsymbol{ heta}_{QP}$	Upper bound solution for $\boldsymbol{\theta}$
$\Theta_l$	$l$ th considered set for $oldsymbol{ heta}$ during optimization
<u>g</u>	Lower bound to the objective function
$\overline{g}$	Lower bound to the objective function

Table S.1: List of symbols used only within the Supplementary Information

<sup>783</sup> The complete optimization problem is written as follows:

$$\hat{\boldsymbol{\beta}}, \hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\beta}, \boldsymbol{\theta}} g(\boldsymbol{\beta}, \boldsymbol{\theta}) = \sum_{j=1}^{J} \sum_{k=1}^{K} \left( \tilde{\boldsymbol{Y}}_{j,k} - \boldsymbol{Y}_{j,k}(\boldsymbol{\beta}) \right)^{2}$$
(S.1)  
s.t.  $\forall k = 1, \dots, K$ :

$$\boldsymbol{Y}(\boldsymbol{\beta}) = \boldsymbol{f}(\boldsymbol{\beta}, \boldsymbol{x}_k)$$
 (S.2)

$$\boldsymbol{\beta} \in \Omega(\boldsymbol{\theta}, \boldsymbol{S}) \tag{S.3}$$

$$\boldsymbol{\theta} \in \boldsymbol{\Theta} \tag{S.4}$$

## 784 S.2.1. Solving for $\beta$

The SCS function fitting problem discussed in the main text is a pseudoconvex program as long as values for the transitions ( $\theta$ ) are fixed and known. Depending on the applied sign constraints and the exact objective function, the problem can be reduced to a semi-definite program, a second order cone program, or even a quadratic program (QP). This is discussed at length in Papp (2011); Villez et al. (2013); Papp and Alizadeh (2014).

## 791 S.2.2. Solving for $\boldsymbol{\beta}$ and $\boldsymbol{\theta}$

The original problem described in the main text requires simultaneous 792 optimization of the transitions  $\boldsymbol{\theta}$ . This is a nonlinear problem. However, and 793 similar to prior work, this kind of problem can be solved to global optimal-794 ity in a deterministic manner by means of the branch-and-bound algorithm 795 (Villez et al., 2013). To this end, the algorithm repeatedly divides the set 796 of feasible values for  $\boldsymbol{\theta}$  ( $\Theta$ ) into smaller subsets until convergence. We refer 797 to the *l*th generated subset during algorithm execution as  $\Theta_l \ (\Theta_l \subset \Theta)$ . For 798 each subset, a lower and upper bound value to the objective function is com-799 puted. These bounds allow ignoring branches in the resulting solution tree 800

during the remainder of the optimization algorithm execution as soon as it is guaranteed that those branches cannot include the global optimum. The exclusion of such branches from the algorithmic search is known as *fathoming*. In what follows, the bounding procedures enabling such fathoming are explained and proven.

<sup>806</sup> S.2.2.1. Step 1: Finding a feasible solution for  $\boldsymbol{\theta}$ . Consider a candidate so-<sup>807</sup> lution set,  $\Theta_l$ . Any such set corresponds to a hyper-rectangular set within <sup>808</sup> the feasible solution space and can be described completely as follows:

$$\boldsymbol{\theta} \in \Theta_l \Leftrightarrow \forall t \in \{1, 2, \dots, T\}: \quad \underline{\theta_t} \le \theta_t \le \overline{\theta_t}$$
(S.5)

with  $\underline{\theta_t}$  and  $\overline{\theta_t}$  describing the interval containing the considered values for  $\theta_t$ .

In addition, each feasible solution within this set satisfies the following order relationship:

$$\forall t \in \{1, 2, \dots, T-1\} : \theta_t \le \theta_{t+1} \tag{S.6}$$

A practical way to propose a feasible solution is obtained by solving the following QP subject to the above conditions (Eq. S.5–S.6):

$$\min_{\boldsymbol{\theta}} \sum_{t=1}^{T} (\theta_t - \underline{\theta_t})^2 + (\theta_t - \overline{\theta_t})^2$$
(S.7)

The solution, if the problem is feasible, is further referred to as  $\theta^{QP}$ . If the set defined by Eq. S.5–S.6 is empty, one cannot find a feasible solution. This case is dealt with separately. <sup>\$18</sup> S.2.2.2. Step 2a: No feasible solution available. When no feasible solution <sup>\$19</sup> for  $\boldsymbol{\theta}$  can be found, the bounding procedures are trivial.

**Procedure.** In this case, the bounding procedures are very straightforward. As in prior work, both the upper bound  $(\overline{g(\Theta_l)})$  and lower bound  $(g(\Theta_l))$  are set to  $+\infty$ :

$$\underline{g} = \underline{g(\Theta_l)} = \overline{g} = \overline{g(\Theta_l)} = +\infty$$
(S.8)

**Proof.** The proof of these bounds is straightforward. Indeed, if no feasible solution can be found  $\theta$ , then there no solution can be found with any objective function value lower than  $+\infty$ . This automatically also defines the upper bound at the same value. This concludes the proof.

<sup>827</sup> S.2.2.3. Step 2b: A feasible solution is found. Computing the upper and <sup>828</sup> lower bounds is more involved when a feasible solution for  $\boldsymbol{\theta}$ , namely  $\boldsymbol{\theta}^{\text{QP}}$ , <sup>829</sup> has been found.

<sup>830</sup> Upper bound – Procedure. An upper bound value for the objective <sup>831</sup> function is computed by replacing  $\boldsymbol{\theta}$  with the proposed solution ( $\boldsymbol{\theta}^{\text{QP}}$ ) in the <sup>832</sup> original problem (Eq. S.1–S.4). This means the following problem is now <sup>833</sup> solved:

$$\hat{\boldsymbol{\beta}}^{\mathrm{U}} = \arg\min_{\boldsymbol{\beta}} \overline{g(\boldsymbol{\beta})} = \sum_{j=1}^{J} \sum_{k=1}^{K} \left( \tilde{\boldsymbol{Y}}_{j,k} - \boldsymbol{Y}_{j,k}(\boldsymbol{\beta}) \right)^{2}$$
(S.9)  
s.t.  $\forall k = 1, \dots, K$ :  
 $\boldsymbol{Y}(\boldsymbol{\beta}) = \boldsymbol{f}(\boldsymbol{\beta}, \boldsymbol{x}_{k})$ (S.10)

$$\boldsymbol{\beta} \in \Omega(\boldsymbol{\theta}^{\mathrm{QP}}, \boldsymbol{S}) \tag{S.11}$$

This problem is again at least pseudo-convex and can thus be solved to deterministic global optimality by means of interior-point algorithms. The corresponding vector containing all spline coefficients is referred to as  $\hat{\boldsymbol{\beta}}^{U}$ . The resulting objective function is an upper bound to the objective function:

$$\exists \boldsymbol{\theta} \in \Theta_l, \exists \boldsymbol{\beta} \in \Omega(\Theta_l, \boldsymbol{S}) : g(\boldsymbol{\beta}, \boldsymbol{\theta}) \le \overline{g} = \overline{g\left(\hat{\boldsymbol{\beta}}^{\mathrm{U}}\right)}$$
(S.12)

<sup>838</sup> Upper bound – Proof. Any feasible solution, including the computed <sup>839</sup> pair ( $\beta^{U}, \theta^{QP}$ ), corresponds to an upper bound as its existence automatically <sup>840</sup> implies that at least one solution exists which delivers an objective function <sup>841</sup> value which is the same or lower value than the computed one,  $g(\beta^{U}, \theta^{QP})$ . <sup>842</sup> As such, this proves the validity of the computed upper bound.

Lower bound – Procedure. A lower bound can be computing by means of the following relaxation of the problem. For the considered subset  $\Theta_l$ , one applies only those sign constraints which are applied universally for all solutions  $\boldsymbol{\theta}$  within the set  $\Theta_l$ . Practically, the original problem is relaxed by replacing the instances of  $\theta_t$  with either  $\boldsymbol{\theta}$  or  $\boldsymbol{\overline{\theta}}$  as follows:

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \underline{g(\boldsymbol{\beta})} = \sum_{j=1}^{J} \sum_{k=1}^{K} \left( \tilde{\boldsymbol{Y}}_{j,k} - \boldsymbol{Y}_{j,k}(\boldsymbol{\beta}) \right)^{2}$$
(S.13)  
s.t.  $\forall k = 1, \dots, K$ :  
 $\boldsymbol{Y}(\boldsymbol{\beta}) = \boldsymbol{f}(\boldsymbol{\beta}, \boldsymbol{x}_{k})$ (S.14)

$$\boldsymbol{\beta} \in \Omega^{\mathrm{L}}(\underline{\boldsymbol{\theta}}, \boldsymbol{\theta}, \boldsymbol{S}) \tag{S.15}$$

where  $\Omega^{L}(\underline{\theta}, \overline{\theta}, S)$  is the relaxed feasible set for  $\beta$ , which is defined as follows:

This relaxed problem is again pseudo-convex and can thus be solved to deterministic global optimality by means of interior-point algorithms. The obtained spline function parameters are referred to as  $\beta^{L}$ . The resulting objective function is a lower bound to the objective function:

$$\forall \boldsymbol{\theta} \in \Theta_l, \forall \boldsymbol{\beta} \in \Omega(\Theta_l, \boldsymbol{S}) : g = g(\boldsymbol{\beta}^{\mathrm{L}}) \le g(\boldsymbol{\beta}, \boldsymbol{\theta})$$
(S.17)

Lower bound – Proof. Because the applied constraints in the modified lower bounding problem are always applied for any particular choice of  $\boldsymbol{\theta}$ for the original problem, one can write that the feasible set for  $\boldsymbol{\beta}$  in the lower bound case,  $\Omega^{L}(\underline{\boldsymbol{\theta}}, \overline{\boldsymbol{\theta}}, \boldsymbol{S})$ , includes the feasible set for any feasible proposal for  $\boldsymbol{\theta}$  for the original problem:

$$\forall \boldsymbol{\theta} \in \Theta_l : \Omega(\boldsymbol{\theta}, \boldsymbol{S}) \subseteq \Omega^{\mathrm{L}}(\underline{\boldsymbol{\theta}}, \overline{\boldsymbol{\theta}}, \boldsymbol{S})$$
(S.18)

Given that the objective function and remaining constraints remain unchanged in the lower bound procedure, it holds that this procedure leads to a proven lower bound. This proves the validity of the lower bound.

S.2.2.4. Bounding gap. In a number of special cases, it can be shown that 862 the lower bound solution will deliver the globally optimal solution within 863 a considered set,  $\Theta_l$ . This is only possible when the considered intervals 864 defining  $\Theta_l$  do not contain any spline basis knot inside their boundaries. 865 Furthermore, this is only guaranteed when the transitions correspond only 866 to changes in the signs of derivatives which are piece-wise linear or piece-wise 867 quadratic in the function's argument. In the case of cubic spline functions, 868 as used in this work, this corresponds to inflection points (2nd derivative is 869 piece-wise linear) and extrema (1st derivative is piece-wise quadratic). This 870

was demonstrated in Villez et al. (2013) for the univariate case (J = 1, K =871 1). This property of the optimization problems means that the bounding gap 872 during branch-and-bound optimization becomes zero in a finite number of 873 steps, leading to absolute precision of the reported globally optimal solution. 874 This property also holds for the extended SCS model studied in this work, 875 however only when the number of considered spline functions is 1 (J = 1,876 without proof). No restrictions are required for the number of measured 877 variables (K, without proof). In the general case  $(J \ge 1)$ , an  $\epsilon$ -optimal 878 solution can be found in a finite number steps, with  $\epsilon$  an arbitrary small 879 strictly positive number. 880

S.2.2.5. Discontinuous trends. Locally discontinuous trends are not consid-881 ered explicitly in this study, unlike Villez and Habermacher (2016). To allow 882 the fitting of SCS functions with discontinuities one only needs to apply the 883 additional relaxations of the optimization problem discussed in Villez and 884 Habermacher (2016) to the multivariate case studied here. This leads again 885 to a valid lower bound (without proof). The upper bound provided in this 886 work remains valid in its current form (without proof). Even though such 887 adjustments are not studied in detail in this work, they are implemented 888 within the provided software toolbox for SCS function fitting. 889

- 890 S.3. Additional figures
- 891 S.3.1. Setup



Figure S.1: Experiment 6 - Image 42. This image is registered with camera 1. The yellow rectangle indicate the selected area for analysis. Camera 2 is visible at the bottom of the image left of the column.





Figure S.2: Experiment 1 – Composite image.



Figure S.3: Experiment  $1 - \text{Composite image with indications of the sludge blanket height identified via shape constrained spline fitting.$ 



Figure S.4: Experiment 1 – Batch settling curve, inflection point, and tangent line obtained with the SCS and MS method for SBH registration.





Figure S.5: Experiment 2 – Composite image.



Figure S.6: Experiment 2 - Composite image with indications of the sludge blanket height identified via shape constrained spline fitting.



Figure S.7: Experiment 2 – Batch settling curve, inflection point, and tangent line obtained with the SCS and MS method for SBH registration.





Figure S.8: Experiment 3 – Composite image.



Figure S.9: Experiment  $3 - \text{Composite image with indications of the sludge blanket height identified via the SCS (yellow) and MS (red) method.$ 



Figure S.10: Experiment 3 - Batch settling curve, inflection point, and tangent line obtained with the SCS and MS method for SBH registration.





Figure S.11: Experiment 4 – Composite image.



Figure S.12: Experiment 4 – Composite image with indications of the sludge blanket height identified via the SCS (yellow) and MS (red) method.



Figure S.13: Experiment 4 - Batch settling curve, inflection point, and tangent line obtained with the SCS and MS method for SBH registration.





Figure S.14: Experiment 5 – Composite image.



Figure S.15: Experiment 5 – Composite image with indications of the sludge blanket height identified via the SCS (yellow) and MS (red) method.



Figure S.16: Experiment 5 – Batch settling curves, inflection points, and tangent lines obtained with all SBH profiles.





Figure S.17: Experiment 6 - Composite image.


Figure S.18: Experiment 6 – Composite image with indications of the sludge blanket height identified via the SCS (yellow) and MS (red) method.



Figure S.19: Experiment 6 – Batch settling curves, inflection points, and tangent lines obtained with all SBH profiles.





Figure S.20: Experiment 7 – Composite image.



Figure S.21: Experiment 7 – Composite image with indications of the sludge blanket height identified via the SCS (yellow) and MS (red) method.



Figure S.22: Experiment 7 – Batch settling curve, inflection point, and tangent line obtained with the SCS and MS method for SBH registration.





Figure S.23: Experiment 8 – Composite image.



Figure S.24: Experiment 8 – Composite image with indications of the sludge blanket height identified via the SCS (yellow) and MS (red) method.



Figure S.25: Experiment 8 - Batch settling curve, inflection point, and tangent line obtained with the SCS and MS method for SBH registration.



Figure S.26: Experiment 9 - Composite image.



Figure S.27: Experiment 9 – Composite image with indications of the sludge blanket height identified via the SCS (yellow) and MS (red) method.



Figure S.28: Experiment 9 - Batch settling curve, inflection point, and tangent line obtained with the SCS and MS method for SBH registration.