Concentration-driven models revisited: towards a unified framework to model settling tanks in water resource recovery facilities

Elena Torfs, M. Carmen Martí, Florent Locatelli, Sophie Balemans, Raimund Bürger, Stefan Diehl, Julien Laurent, Peter A. Vanrolleghem, Pierre François and Ingmar Nopens

ABSTRACT

A new perspective on the modelling of settling behaviour in water resource recovery facilities is introduced. The ultimate goal is to describe in a unified way the processes taking place both in primary settling tanks (PSTs) and secondary settling tanks (SSTs) for a more detailed operation and control. First, experimental evidence is provided, pointing out distributed particle properties (such as size, shape, density, porosity, and flocculation state) as an important common source of distributed settling behaviour in different settling unit processes and throughout different settling regimes (discrete, hindered and compression settling). Subsequently, a unified model framework that considers several particle classes is proposed in order to describe distributions in settling behaviour as well as the effect of variations in particle properties on the settling process. The result is a set of partial differential equations (PDEs) that are valid from dilute concentrations, where they correspond to discrete settling, to concentrated suspensions, where they correspond to compression settling. Consequently, these PDEs model both PSTs and SSTs.

Key words | compression, discrete settling, primary clarifier, secondary clarifier, settling velocity distribution

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INTRODUCTION

In the conventional treatment of wastewater, both primary settling tanks (PSTs) and secondary settling tanks (SSTs) aim at separating suspended particles from the liquid phase through sedimentation. Although both unit processes are based on the same principle, i.e. settling due to gravity, the modelling approaches have been markedly different. SSTs have been modelled by a single concentration variable for the particle phase (Takács *et al.* 1991; Plósz *et al.* 2007; Bürger *et al.* 2013), which means that this phase is considered as a continuum, as is the liquid phase. Hence, all particles are indirectly assumed to be identical. We call this a concentration-driven model. In contrast, discrete

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settling in PSTs and the clarification zone of SSTs is known to be governed by distributed settling dynamics driven by individual particle properties (e.g. size, density, shape). However, as the segregation between particles differing in size, density or shape is challenging to model, the clarification process in SSTs is generally lumped into concentration-driven models (by introducing an additional term in the hindered settling velocity function to describe low concentrations) (Takács *et al.* 1991) and PSTs have mostly been described by simplified models (using linear regression to relate the removal efficiency to certain characteristics of the incoming wastewater) (Amerlinck 2015).

With current focus shifting towards recovery of energy and resources, new challenges arise for operation and control of water resource recovery facilities (WRRFs). This also stimulates a renewed interest in settling as separation process as the separation of interesting fractions is an obvious first step towards their recovery. For PSTs, recent advances have led to a more detailed model based on a number of particle classes with different settling velocities (Bachis *et al.* 2015). This model is called the particle settling velocity distribution (PSVD) model and allows the simulation of distributed settling of the incoming wastewater particles. On the other hand, more advanced concentration-driven models for SSTs have gained increased attention (Kinnear 2002; Plósz *et al.* 2007; De Clercq *et al.* 2008; Bürger *et al.* 2013; Li & Stenstrom 2014). The focus here has been on the incorporation of compression (i.e. the resistance to hindered settling by the network of flocculated particles that arises at high concentrations) as several studies have shown that hindered settling alone does not capture the complex settling behaviour of activated sludge (De Clercq *et al.* 2005; Ramin *et al.* 2014; Torfs *et al.* 2015). Although compression settling is known to depend on the concentration gradient, which introduces a second-order term in the governing partial differential equation (PDE), the exact relation describing this compressive behaviour is still unknown. A number of studies proposed expressions to describe compression from experimental data (De Clercq *et al.* 2008; Ramin *et al.* 2014; Diehl 2015). However, these analyses evidenced that identification of a compression function in a purely concentration-driven model was not possible as the physics of compression cannot be modelled only in dependence of the concentration X (and its gradient) with a constant parameter set. Some approaches introduce an empirical variation in the transition concentration between hindered and compression settling (the so-called critical concentration X_{crit}) (De Clercq *et al.* 2008; Ramin *et al.* 2014; Locatelli 2015) but a physical explanation for this variability has not yet been provided.

The first part of this contribution provides new experimental evidence that the unexplained variability in thickening and compression behaviour in SSTs has a similar origin as the variability observed in PSTs and the clarification zone of SSTs. Variations in distributed particle properties such as size, shape, porosity, density and flocculation state leading to a distributed settling velocity are shown to have an important influence on the settling behaviour in different settling unit processes (and at different concentrations throughout these unit processes). Hence, although each settling process is still governed by its own specific dynamics, these dynamics can be attributed to a common source, thus calling for a unified framework to describe the different settling unit processes. The experimental evidence presented in this first part provides the background and motivation for the second part of this contribution which addresses the development of a unified settling framework. The conceptual steps to extend current models into a framework that can be applied to different settling unit processes are presented. Finally, in a third part, the potential of the new proposed framework is illustrated with simulation examples.

EXPERIMENTAL EVIDENCE IN SUPPORT OF A UNIFIED FRAMEWORK

Discrete settling in PSTs and the clarification zone of SSTs

Discrete settling in the clarification zone of SSTs is often modelled by directly modifying classical concentration-based hindered settling velocity functions. Unfortunately, this approach is not sufficiently generic for reliable effluent suspended solids predictions since it cannot capture the true (distributed) settling behaviour using a single parameter set. Figure 1 illustrates the behaviour of secondary sludge at low concentrations (approx. 500 mg/L). Several samples were taken at the top of a settling column during the settling process and the particle size distribution (PSD) of each was measured by image analysis with an Eye-Tech particle size analyser (Ankersmid, The Netherlands) (Torfs 2015). As time increases, larger particles are no longer observed in the PSD, indicating that particles of different sizes settle sequentially. These results confirm that settling at low concentrations is governed by distributed properties such as particle size and density. Moreover, Bachis *et al.* (2015)

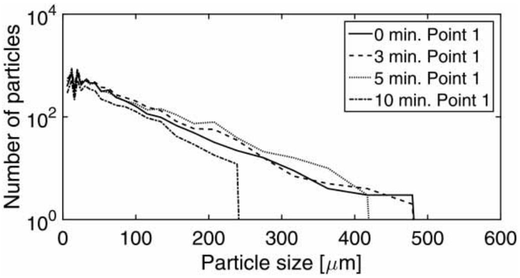

Figure 1 | Example of clarification behaviour in SSTs. Changes in PSDs at the top of a settling column for a diluted (approx. 500 mg/L) sludge sample (Torfs 2015).

used the ViCAs protocol (Chebbo & Gromaire 2009) to measure PSVDs during batch settling of raw wastewater (Figure 2). These results clearly indicate that the settling in PSTs and the clarification zone of SSTs demonstrates a distributed behaviour whose dynamics cannot be captured by a lumped variable such as concentration.

Hindered and compression settling in the thickening zone of SSTs

Hindered and compression settling have traditionally been considered as concentration-driven processes where the settling velocity decreases with increasing concentration. However, this approach is not sufficient to explain recent experimental observations. Figure 3 illustrates the evolution of the sludge blanket height (and thus the settling velocity at the top of the sludge blanket) for batch settling experiments under different conditions. Figure 3 (left) shows changes in settling behaviour after addition of loess (density $\rho \approx 1.7$ kg/L) (Locatelli 2015). Although the addition of loess will increase the concentration of suspended solids, the settling velocity increases. This contradicts conventionally

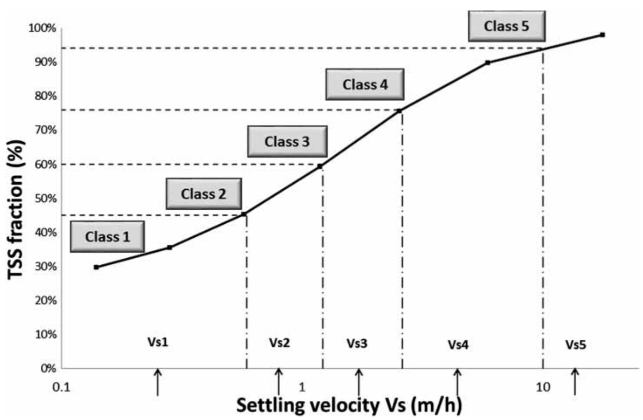

Figure 2 | Example of settling behaviour in PSTs. Settling velocity distribution during settling of raw wastewater (Bachis *et al.* 2015).

used models for hindered and compression settling that would predict the opposite tendency. Variations in sludge density are thus shown to play an important role next to concentration.

Figure 3 (right) shows how the settling behaviour of a sludge sample changes as it is subject to different amounts of shear stress prior to settling. The settling velocity at the top of the sludge blanket changes noticeably between the different experiments. Since each of these tests was performed at the same initial concentration, the differences in settling behaviour cannot be attributed to variations in concentration but only to variations in particle properties. By stirring the sample, the flocculation state of the sludge is changing as loosely bound flocs are broken up into more stable aggregates. This process may be further facilitated by the release of extracellular polymeric substances acting like a polymer to increase flocculation (Laurent *et al.* 2009). The resulting aggregates are characterised by better settling properties leading to a faster decrease in the sludge blanket height. Stirring the sample at high shear rates also decreased the sludge's ability to act as a filter for colloids, causing an increase in supernatant turbidity.

Moreover, Figure 3 (right) illustrates the impact of variations in particle properties with respect to the onset of compression settling. For suspensions with sufficiently low critical concentration X_{crit} (such as activated sludge), the bend in the batch settling curve corresponds to the point where the sludge blanket enters the compression zone. (Note that for suspension of, for example, hard spherical particles, that undergo hindered settling only, such a bend may also occur, but this does not apply here.) Hence, for the curves in Figure 3 (right) the onset of compression is indicated by the grey dotted lines. At these points, the concentration at the top of the sludge blanket should equal the critical concentration. When shear is applied prior to settling, the sludge water interface reaches the compression zone earlier and, more importantly, at a much lower sludge blanket height (and thus in a more concentrated state). A more concentrated sludge blanket at the onset of the compression zone signifies a higher critical concentration. This indicates that differences in distributed particle properties potentially account for variations in the critical concentration. Due to the applied shear, larger and less stable flocs will be reduced to smaller and denser flocs with different packing properties resulting in a sample that can reach higher concentrations before the particles are in permanent contact.

The combined results of Figure 3 indicate that similar to settling at low concentrations, changes in size, shape and

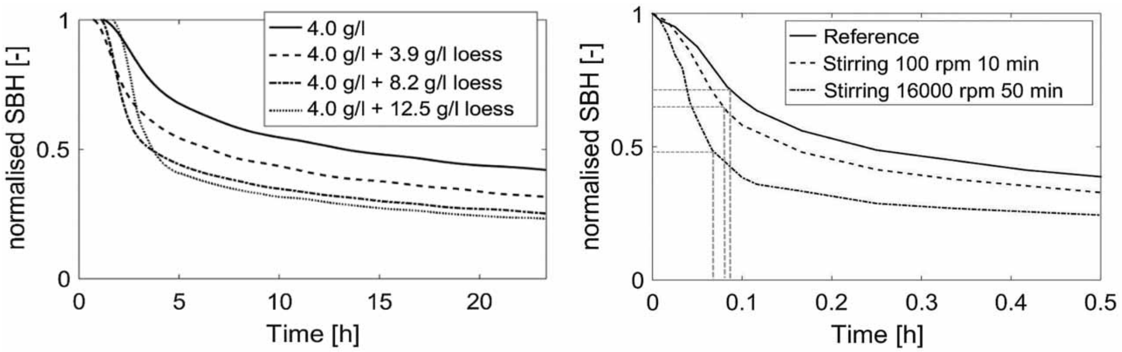

Figure 3 | Normalized sludge blanket height observed in batch settling experiments for a sludge sample which has been subjected to different amounts of loess addition (Locatelli 2015) (left) and different amounts of shear stress (right).

density should also be considered as important factors to describe the variability in hindered and compression settling. This finding has important implications for the modelling of settling processes as it emphasizes the need to step away from purely concentration-driven SST models and opens up new perspectives for a unified settling framework which can be applied to all settling unit processes.

New applications of a unified model framework

A unified framework which can capture the true variability in the settling behaviour would allow expanding the use of settler models beyond their current applications. For conventional SSTs this would not only allow improved predictions of effluent suspended solids but also to model the impact of chemical addition and increased hydraulic loadings. For PSTs, this would allow to model compression of the particles accumulated at the bottom to better predict the underflow concentration (and consequently the feed concentration to an anaerobic digester).

Moreover, a number of emerging technologies for WRRFs could also benefit from such improved settler models. For example, high-rate activated sludge processes receive increased interest due to their capability to efficiently concentrate organics into a well-digestible sludge (Verstraete & Vlaeminck 2011). The specific process conditions impact the size, shape and density of the flocs which have important implications for the settling behaviour in these systems. This is illustrated in Figure 4 where batch settling curves for conventional activated sludge from the WRRF of Destelbergen (Belgium) are compared to batch settling curves for sludge from a laboratory-scale high-rate contact stabilisation (HiCS) reactor (Meerburg *et al.* 2015). A significant difference in the settling behaviour of the two systems can be observed. The settling curves of the two highest concentrations of the conventional sludge (5.46 g/L and 6.83 g/L respectively) show very poor settling properties. The absence of an initial linear descent in these curves means that compression is present from the start of the settling experiment. The critical concentration will thus be smaller than 5.46 g/L. For the settling curves of the sludge of the HiCS reactor a clear linear descent is present up to a concentration of 8.5 g/L, indicating that $X_{crit} > 8.5$ g/L. This sizeable difference in compression behaviour can be attributed to the combination of a very short solids residence time in combination with a feast–famine regime in the HiCS reactor. Such growth conditions are known to have an advantage for floc-formers (Guo *et al.* 2014) resulting in small and dense flocs with good settling and compaction properties. A similar principle can be observed in selectors for the prevention of bulking sludge (Forster 1996). These observations emphasize again that a framework that includes information on individual particle properties is highly desirable as such models will, for instance, facilitate the development of strategies for energy recuperation from settled solids leading to more energy-efficient wastewater treatment.

DEVELOPMENT OF A UNIFIED SETTLING MODEL FRAMEWORK

Current state of the art settling models

From the examples above, distributed properties such as particle size, shape and density were shown to be key factors in describing the settling processes in WRRFs. Existing secondary settling models such as the traditional Takács model (Takács *et al.* 1991) and the more recent Bürger-Diehl framework (Bürger *et al.* 2013) do not account for distributed

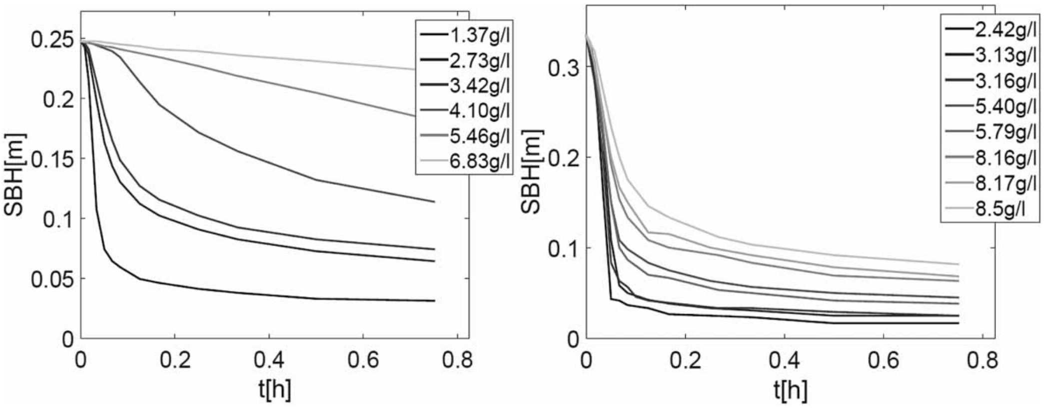

Figure 4 | Comparison of batch settling curves at different initial TSS concentrations for conventional activated sludge from the WWTP of Destelbergen, Belgium (left) and sludge from a laboratory-scale HiCS-reactor (right).

behaviour of particles; they simply describe the solids by means of a lumped concentration variable. Moreover, neither of these settling models consider changes in particle properties due to aggregation and break-up processes. Empirical relations describing the effect of polymer addition on hindered settling have been described in literature (Vanderhasselt *et al.* 1999) but these do not account for the underlying changes in particle property distributions. Recently, a new model for PSTs, called the PSVD model (Bachis *et al.* 2015), was presented. The PSVD model does include distributed settling behaviour and has been extended to include the effect of chemically enhanced primary treatment (CEPT) by alum dosage (Tik *et al.* 2016). However, this model only covers the discrete settling regime and can therefore not be applied to SSTs.

In order to achieve a unified description of the processes taking place both in PSTs and SSTs, either existing PST models such as the PSVD have to be extended with hindered and compression dynamics or existing SST models need to be extended to include particle classes and their associated distributed behaviour. In this contribution, it was chosen to start from the existing Bürger-Diehl framework for SSTs (Bürger *et al.* 2013) as this framework already includes hindered and compression settling in its underlying PDE and most importantly an appropriate numerical scheme to solve this PDE. The Bürger-Diehl framework can be further extended by combining knowledge from several existing approaches. These include the PSVD model in PSTs but can also be found outside WWT modelling such as models for polydisperse sedimentation (Berres *et al.* 2003) and population balance models (PBMs) describing the mechanisms of flocculation and breakage (Nopens *et al.* 2015). The remainder of this contribution provides the conceptual steps to extend the Bürger-Diehl framework into a unified framework for the settling dynamics in different settling unit processes.

The Bürger-Diehl secondary settler framework

The model equation is the following PDE for the local concentration X:

$$\begin{aligned}\frac{\partial X}{\partial t} = &-\frac{\partial}{\partial z}(v_b(z,t)X) && \text{bulk flow}\\ &-\frac{\partial}{\partial z}(v_{hs}(X)X) && \text{hindered settling}\\ &+\frac{\partial}{\partial z}\left(d_{comp}(X)\frac{\partial X}{\partial z}\right) && \text{compression settling}\\ &+\frac{Q_f(t)X_f(t)}{A}\delta(z) && \text{incoming feed flow}\end{aligned} \tag{1}$$

Here, Q_f is the incoming feed flow rate, X_f the feed flow concentration, A the surface area and z the depth measured from the feed inlet. The feed inlet at $z = 0$ is modelled as a point source with the delta Dirac function $\delta(z)$. The phenomenon of dispersion at the inlet is not considered – this is not the focus here and it can be included at a later stage. The bulk velocity v_b depends on z, since the inlet flow is divided into the upward/downward flows in the clarification/thickening zones. The hindered settling velocity $v_{hs}(X)$ and compression function $d_{comp}(X)$ have the following forms:

$$v_{hs}(X) = v_0 v(X) \tag{2}$$

$$d_{comp}(X)\begin{cases} = 0 & \text{for } 0 \leq X \leq X_{crit} \\ > 0 & \text{for } X > X_{crit}\end{cases} \tag{3}$$

where v_0 is the maximum settling velocity for a single particle and $v(X)$ which should satisfy $v(0) = 1$, can represent any hindered settling function from literature (exponential, power-law, rational…) (Vesilind 1968; Takács *et al.* 1991; Cho *et al.* 1993; Diehl 2015). For example, for the Vesilind expression we have $v(X) = \exp(-r_V X)$. The parameter X_{crit} is the critical concentration above which the sludge forms a network that can be compressed and d_{comp} is a compression function (De Clercq *et al.* 2008; Ramin *et al.* 2014).

The total flux of solids in the settling tank is thus dependent on bulk flow, hindered settling and compression settling and can be written as:

$$F\left(X, \frac{\partial X}{\partial z}, z, t\right) = \underbrace{\left(v_{\mathrm{b}}(z, t) + v_{\mathrm{hs}}(X) - \frac{d_{\mathrm{comp}}(X)}{X}\frac{\partial X}{\partial z}\right)}_{\text{velocity of solids movement}} X. \tag{4}$$

In order to obtain a unified modelling framework that can describe the effect of changes in particle property distributions on the settling behaviour, the following specific changes/additions need to be made to the Bürger-Diehl framework.

1. A number of classes needs to be introduced to represent the distributed properties of the sludge.
2. These different classes allow to extend the existing framework with distributed settling behaviour such as discrete settling and to account for the effect of distributed particle properties on hindered and compression dynamics.
3. The model equations can also be augmented with reaction terms to describe changes in particle property distributions due to operational and loading conditions. These different steps are introduced below.

Extension to several particle property classes

The distributed properties of the sludge can be captured by dividing the total sludge concentration X amongst a number of particle classes based on either size, density (or a combination of the former) or directly on settling velocity distributions depending on the available knowledge and data. Hence,

$$X = \sum_{i=1}^{n} X_i \tag{5}$$

for n particle classes each having a certain concentration X_i.

A well-flocculated sludge will have a larger concentration of particles in the large/dense/fast class and a lower concentration of particles in the class of small/open/slow particles.

Instead of a single nonlinear convection-diffusion PDE, this will result in a system of PDEs, one for each particle property class. Such a set of PDEs has been presented in literature (Berres *et al.* 2003) for classes of particles having different sizes and densities. In its most general treatment, each particle class has its own settling velocity function which depends on the concentrations of all classes and their spatial derivatives, making it quite complex. Therefore, in this work, a simpler approach is followed, where only a number of specific dependencies required to capture the dynamics of settling in WRRFs are added.

As a first step, we maintain the assumption that hindered and compression settling are functions of the total sludge concentration. Hence, particles of all classes will settle at the same velocity and we only need to redistribute the total flux (Equation (4)) over the different particle classes. Although this may seem trivial, the distribution of the flux over different classes is essential for further model extension with discrete settling and flocculation processes in the next steps. The following can then describe the flux in class $i = 1,\ldots,n$:

$$F_i\left(X, \frac{\partial X}{\partial z}, X_i, z, t\right) = \left(v_{\mathrm{b}}(z, t) + v_{\mathrm{hs}}(X) - \frac{d_{\mathrm{comp}}(X)}{X}\frac{\partial X}{\partial z}\right) X_i \tag{6}$$

and the system of PDEs modelling the changes in concentration for all classes will have the following form:

$$\frac{\partial X_i}{\partial t} = -\frac{\partial}{\partial z} F_i\left(X, \frac{\partial X}{\partial z}, X_i, z, t\right) + \frac{Q_{\mathrm{f}}(t) X_{\mathrm{f},i}(t)}{A}\delta(z), \quad i = 1, \ldots, n \tag{7}$$

with $X_{\mathrm{f},i}$ the concentration of class i in the feed flow. Once a system of PDEs describing the change in concentration for different classes is defined, certain class-dependent processes can be specified, such as distributed settling behaviour and reaction terms to describe the migration of particles between the different classes (i.e. flocculation and break-up).

Specification of distributed settling behaviour

At low concentrations such as those occurring in the PST or in the clarification zone of the SST, sludge particles typically undergo discrete settling. As the discrete settling velocity is considered independent of concentration, each particle class will settle at its own characteristic velocity ($v_{0,i}$).

Moreover, recent experimental evidence (Locatelli *et al.* 2015) revealed that also during the hindered settling regime, the settling velocity of flocculated particles exhibits distributed behaviour (Figure 5). This result was not expected as, according to the prevailing definition of hindered settling, all particles in this regime are expected to settle at the same velocity determined by the initial concentration in the batch reservoir. Such behaviour would generate a more or less vertical line in the settling velocity profile of the hindered settling region. However, the large fluctuations in the settling velocity observed throughout the hindered settling regime in Figure 5 (left) show that this is clearly not the case. In contrast, the settling velocity is noticeably distributed over a large interval of velocities. These observed fluctuations, and thus the width of the settling velocity distribution, decreases with increasing concentration (Figure 5 – right). Once the sludge reaches the compression region, hardly any fluctuations can be observed. It can thus be assumed that the compression function shows no distributed behaviour but will only depend on the local concentration X and its derivative.

The distributed dynamics for discrete settling and the decreasing distributed behaviour during hindered settling can be included in the model framework with the following 'discrete-hindered-settling' velocity function (to be used instead of Equation (2)):

$$v_{\text{dhs},i}(X) = \begin{cases} v_{0,i} & \text{if } X < X_{\text{trans}} \\ v_{0,i} v(X - X_{\text{trans}}) & \text{if } X \geq X_{\text{trans}} \end{cases} \tag{8}$$

The parameter $X_{\text{trans}} \geq 0$ represents the transition concentration between discrete and hindered settling.

The corresponding behaviour of the function $v_{\text{dhs},i}(X)$ is illustrated in Figure 6. At concentrations below the transition concentration X_{trans}, the settling behaviour in each particle property class i is governed by its discrete settling velocity $v_{0,i}$ independent of the overall concentration (Figure 6 – left) and the settling velocity over the different classes shows its maximum distribution (Figure 6 – right). As the concentration increases ($X \geq X_{\text{trans}}$), the particles will start to hinder each other's settling behaviour. Hence, the settling velocity decreases and the distribution of settling velocities becomes narrower until, at high concentrations (5.9 g/L for the example in Figure 6), all particle classes have approximately the same settling velocity. This gradual reduction in distributed behaviour corresponds to the observations made from the experimental data of Locatelli *et al.* (2015) in Figure 5.

For the example presented in Figure 6, the transition between discrete and hindered settling causes an abrupt

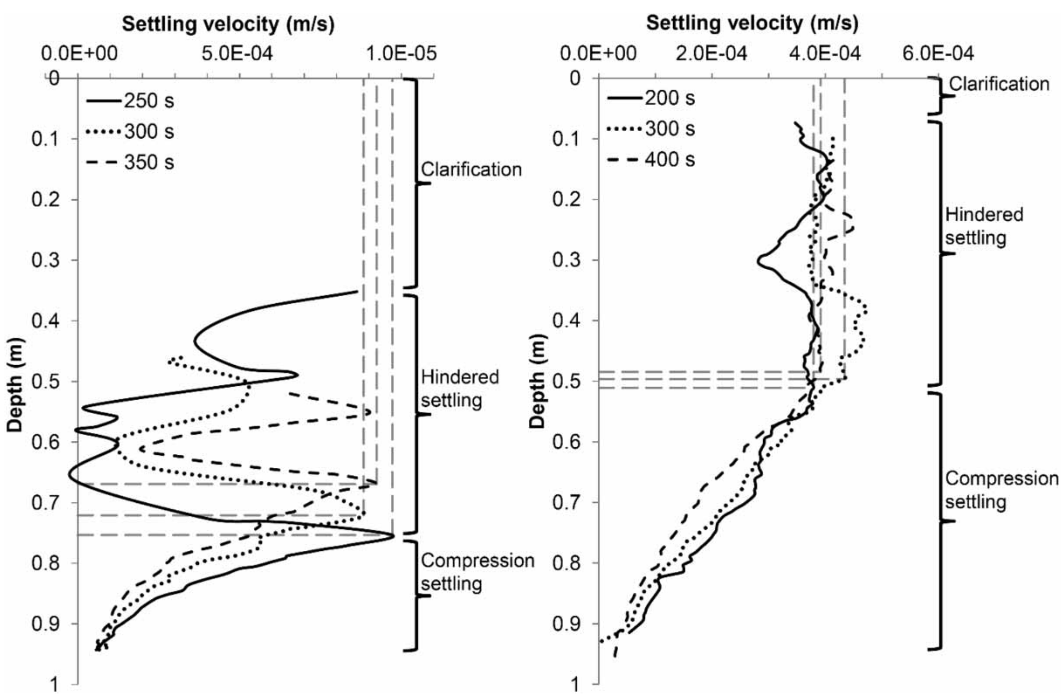

Figure 5 | Settling velocity profiles recorded with an ultrasonic transducer during batch settling at an initial concentration of 1.5 g/L (left) and 4.6 g/L (right) (Locatelli *et al.* 2015).

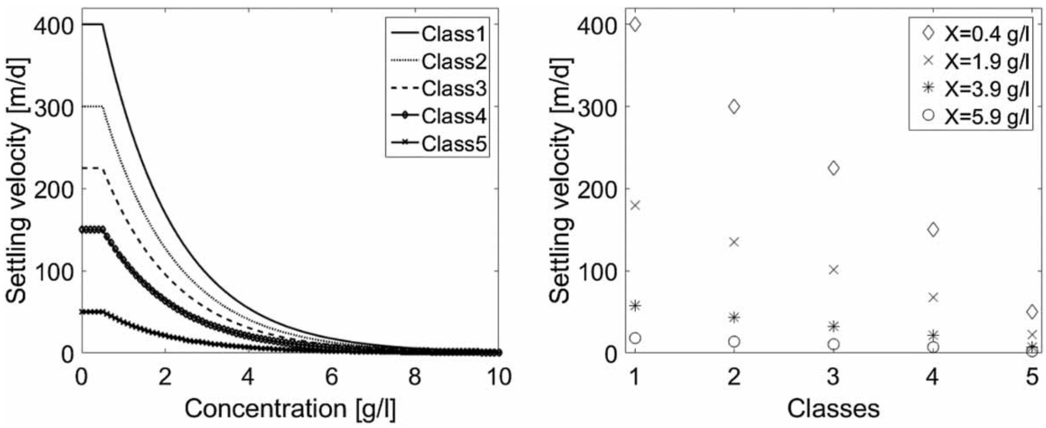

Figure 6 | Example of settling velocity in function of concentration for different particle property classes (left) and the corresponding change in settling velocity distribution with increasing concentration (right). For this example the exponential hindered settling velocity function of Vesilind (1986) was used.

change in settling behaviour which may feel counter intuitive from a physical perspective. This abrupt change is a specific feature of the exponential hindered settling function of Vesilind (1986) that was selected for this example. Alternative hindered settling functions that allow a smooth transition between the two settling regimes are also available in the literature such as the rational function by Diehl (2015):

$$v(X) = \frac{1}{1 + (X/\bar{X})^q} \quad (9)$$

where $\bar{X}$ and q are constants.

When the function (8) is used to describe discrete and hindered settling, the total flux function for class i becomes (to be used instead of (6))

$$F_i\left(X, \frac{\partial X}{\partial z}, X_i, z, t\right) = \left(v_\mathrm{b}(z, t) + v_{\mathrm{dhs},i}(X) - \frac{d_{\mathrm{comp},i}(X)}{X}\frac{\partial X}{\partial z}\right)X_i. \quad (10)$$

We write here $d_{\mathrm{comp},i}(X)$ instead of $d_{\mathrm{comp}}(X)$ since compression is considered as a force working against gravitational settling (De Clercq *et al.* 2008) which changes between particle classes through the definition of Equation (8).

By substituting Equation (10) in Equation (7), the corresponding set of PDEs is valid from dilute concentrations ($X < X_{\mathrm{trans}}$), for which they coincide with discrete settling models, to concentrated suspensions ($X > X_{\mathrm{crit}}$) in which the sediment is described as a permanently networked, compressible porous layer. It can thus be used to model both PSTs and SSTs.

The distributed properties of the sludge will not only cause distributed settling behaviour but will also influence the transition between the different settling regimes (characterised by X_{trans} and X_{crit}). For example, aerobic granular sludge is known to have a low tendency to coagulate under reduced hydrodynamic shear (de Kreuk & van Loosdrecht 2004). This feature causes granular sludge to undergo discrete settling at concentrations where conventional activated sludge experiences hindered or compression settling. The presented framework can be applied to granular sludge by simply setting an appropriately high transition concentration X_{trans}.

As a second example, the impact of changes in particle property distributions with respect to the onset of compression settling (characterized by a bend in the batch settling curve) is illustrated in Figure 3 (right) and Figure 4. When shear is applied prior to settling (Figure 3 – right) or when more floc-formers are present, as was the case for the example of HiCS sludge in Figure 4, the sludge-water interface reaches the compression zone at a much lower height (and thus in a more concentrated state). A more concentrated sludge blanket at the onset of the compression zone indicates a higher critical concentration. A reasonable way to define the relation between the critical concentration and the distributed particle properties could be the following:

$$X_{\mathrm{crit}}(X_1 \ldots X_N) = \sum_{i=1}^{N} \frac{X_i}{X} X_{\mathrm{crit},i} \quad (11)$$

In this function $X_{\mathrm{crit},i}$ corresponds to the critical concentration that would arise in a suspension of mono-sized particles of class i. The total critical concentration of a mixture of different particle classes is calculated (at each height in the settling column and each simulation time) as a weighted sum of $X_{crit,i}$ according to the concentration of each particle class present. The reasoning behind this definition stems from the idea that faster settling particles (for example the HiCS sludge in Figure 4) would have a less porous structure thus allowing for a denser packing before being subjected to the force of compression. As such, the proposed modelling framework is able to describe the unexplained variability in the critical concentration (reported by De Clercq *et al.* (2008) and Ramin *et al.* (2014)) through changes in distributed particle properties. A similar approach can be applied to define the transition between discrete and hindered settling (X_{trans}) as a weighted function of the concentrations in the different classes.

Specification of flocculation processes

The equations presented above allow modelling the effect of changes in particle properties of the incoming feed flow (through $X_{f,i}$(t)). In order to incorporate the effect of changes in operational and load conditions on the particle property distribution, these equations can be further extended with reaction terms r describing flocculation/break-up processes. As the main factors influencing flocculation and break-up are shear and the addition of chemicals, the reaction rates will (mainly) depend on the incoming flow rate, the settler's configuration (e.g. baffles) and concentration of chemicals (C_{chem}).

$$\frac{\partial X_i}{\partial t} = -\frac{\partial}{\partial z} F_i\left(X, \frac{\partial X}{\partial z}, X_i, z, t\right) + \frac{Q_f(t) X_{f,i}(t)}{A}\delta(z) + r_i(Q_f, X_i, X, C_{chem}), \quad i = 1, \ldots, n \tag{12}$$

The reaction terms $r_i(Q_f, X_i, X, C_{chem})$ can be based on flocculation jar experiments (Gong *et al.* 2011) or can be derived from PBMs which allow detailed modelling of the dynamics of distributions (Nopens *et al.* 2015).

An alternative and simple approach would be to assume that flocculation/break-up is mostly occurring in the flocculation well. In this case, the flocculation well can be described as a continuous stirred tank reactor (CSTR) prior to the actual settling tank where flow dependent flocculation and break-up processes give rise to a certain particle class distribution that can subsequently be fed as input to the one-dimensional (1D) settler model. This approach would remove the need to add reaction terms to each PDE. However, it is only valid for well-designed clarifiers where flocculation is indeed (approximately) limited to the flocculation well.

SIMULATION EXAMPLE

This section presents a simulation example to illustrate the specific features of the proposed unified model framework emphasizing its ability to describe variability in settling behaviour that cannot be attributed to changes in concentration only. The model equations were implemented for batch sedimentation only (no bulk flow nor incoming feed flow), and flocculation between classes is not considered thus far ($r_i = 0$). The example includes all three settling regimes (discrete, hindered and compression settling) with discrete and hindered settling velocity functions given by Equation (8).

Introducing different particle classes in a settler model gives rise to a number of coupled second-order PDEs whose discretization might pose significant restrictions on the time step of the solution. Moreover, due to the nature of settling as a separation process, simulation results will give rise to sharp discontinuities in the concentration profiles of all classes. To handle these issues, an IMEX scheme (Boscarino *et al.* 2015) was used for the numerical implementation of this system. In this scheme, first-order convection terms are discretised in an explicit way and second order diffusive terms are handled in a linearly implicit way ensuring an efficient solution of the proposed model framework. All details concerning the application of an IMEX scheme to the presented model framework can be found in Bürger *et al.* (in preparation).

The specific constitutive functions used for hindered and compression settling were defined by:

$$v_{dhs,i}(X) = \begin{cases} v_{0,i} & \text{if } X < X_{trans} \\ v_{0,i}\exp(-r_H(X - X_{trans})) & \text{if } X \geq X_{trans} \end{cases} \tag{13}$$

$$d_{comp,i}(X) = \begin{cases} 0 & \text{if } X < X_{crit}(X_1 \ldots X_N) \\ \dfrac{\rho_s \alpha v_{dhs,i}(X)}{g(\rho_s - \rho_f)} & \text{if } X \geq X_{crit}(X_1 \ldots X_N) \end{cases} \tag{14}$$

Hindered settling is expressed as an exponentially decaying function (with settling parameter $r_H = 0.45\ m^3/kg$) and compression as a function of solid and liquid densities ($\rho_s = 1{,}050\ kg/m^3$, $\rho_f = 998\ kg/m^3$), and a compression parameter α ($\alpha = 0.5\ m^2/s^2$). The transition concentration between discrete and hindered settling X_{trans} was set to a constant value of 1 kg/m^3. The total critical concentration, on the other hand, was modelled as a function of the particle distribution according to Equation (11). For the simulations presented in this section, the total sludge concentration was divided into 10 particle classes according to their settling velocity distribution. Table 1 shows the discrete settling velocities and critical concentrations that were used for the different particle classes. The values for discrete settling velocity were based on settling velocity distribution measurements (Tik *et al.* 2016), whereas the critical concentrations were allowed to vary linearly in a range based on observations made by De Clercq *et al.* (2008).

Simulations of a batch settling experiment were performed with a uniform initial concentration of 4 g/L. The effect of distributed particle properties on settling behaviour was analysed by varying the initial distribution over the 10 particle classes. Three different scenarios at different initial particle distributions were considered (see Figure 7). In a first scenario, the total concentration is divided over the different classes according to a normal distribution. A second scenario considers a distribution shifted slightly to the left corresponding to the presence of more slowly settling particles which can, for example, be caused by the presence of excessive filaments. In the last scenario, the distribution is shifted slightly to the right thus including more fast settling particles (e.g. through the addition of a flocculant).

Figure 8 shows the simulated sludge blanket heights for the three scenarios over 30 min of settling. It can clearly be seen that, although for each scenario the settling column was filled with the same uniform concentration, the differences in initial distribution (Figure 7) cause distinctly different settling behaviour. The sludge blanket for the left-biased distribution settles slowest due to the larger presence of slower settling particles than the other scenarios. It should be stressed that traditional concentration-based SST models are unable to capture this behaviour without recalibrating the hindered and/or compression settling functions.

More detailed information on the model's behaviour can be deduced from Figure 9. Here, the concentration profiles over the depth of the settling column are shown for the first and second scenario (normal distribution – left and left-biased distribution – right). The top graphs show the concentration profiles of the total concentration (in black) after 5 min of settling whereas the bottom graphs show the concentration profiles after 20 min. These concentration profiles indicate that not only the predictions of the sludge blanket heights are influenced by the distributed particle properties but also the concentration at the bottom of the batch reservoir are markedly different

Table 1 | Definition of critical concentration ($X_{crit,i}$) and discrete settling velocity ($v_{0,i}$) for each particle class

	Particle class									
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
$X_{\mathrm{crit},i}$ [kg/m^3]	8	8.66	9.33	10	10.66	11.33	12	12.66	13.33	14
$v_{0,i}$ [m/d]	5	20	70	150	300	500	800	1,300	2,000	4,500

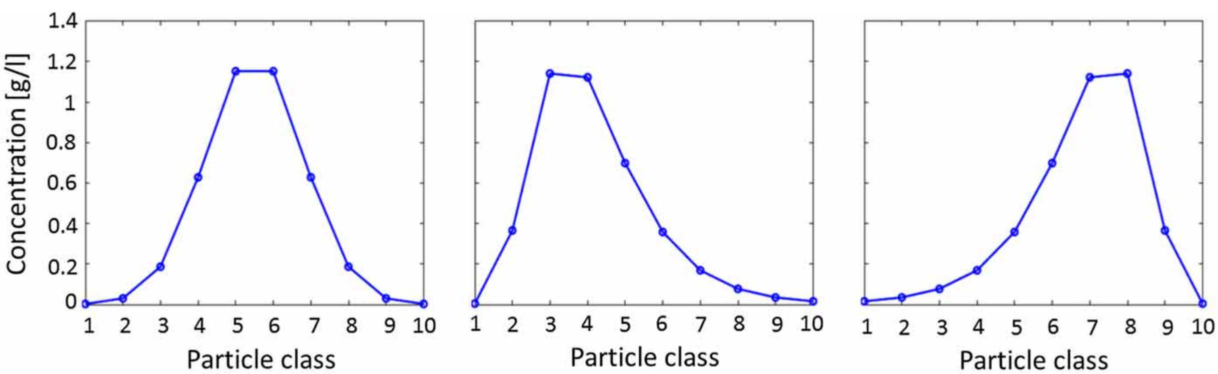

Figure 7 | Three different distribution functions to represent sludge suspensions with the same concentration but different particle properties.

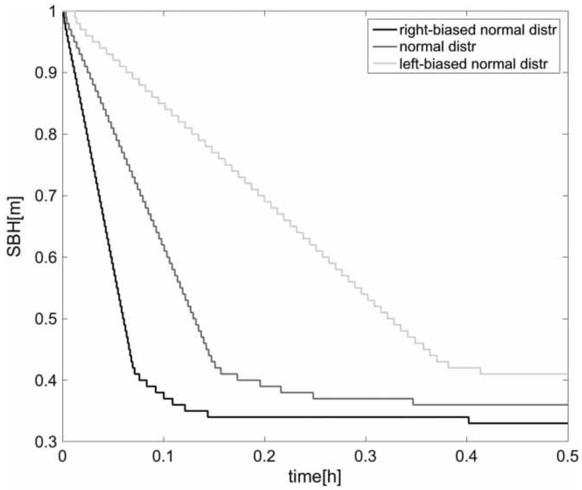

Figure 8 | Sludge blanket heights during batch settling of a mixture with a total concentration of 4 g/L as predicted by the unified model framework for the different initial distributions of Figure 7.

between the two scenarios. The distributed discrete and hindered settling velocity (see (13)) in the proposed model framework allows for a segregation of particles over the length of the column. Faster settling particles will preferentially make up the bottom layers, whereas very slow settling particles remain much longer in the supernatant. This segregation of particles also influences the value of the critical concentration (defined by Equation (11)) thus allowing variations in initial particle properties to influence the compression behaviour in the sludge blanket. As such, the variability in sediment compressibility (which has been previously reported but never supported by a physical explanation) can be captured, allowing for a more detailed description of the build-up of the sludge blanket. Further discussion of the phenomena observed in the obtained concentration profiles is out of scope of this contribution.

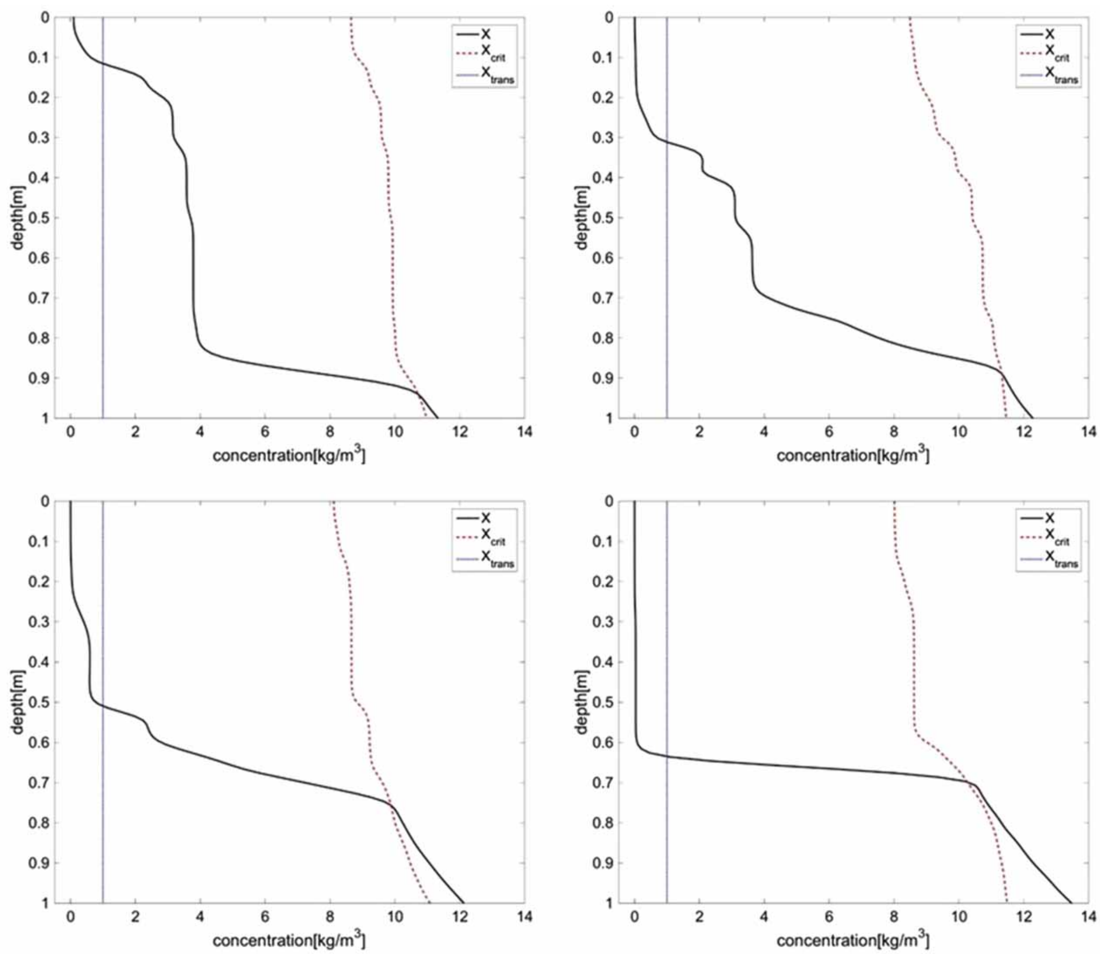

Figure 9 | Concentration profiles over the depth of the settling column for a normal initial particle distribution (left) and a left-biased initial particle distribution (right). The top graphs show the concentration profiles after 5 min of settling whereas the bottom graphs show the concentration profiles after 20 min.

CONCLUSIONS

Experimental evidence of sludge settling at different concentrations and under different conditions showed that variations in distributed particle properties (such as size, shape, porosity and density leading to a distributed settling velocity) are an important factor influencing the settling behaviour in all settling unit processes in WRRFs. Hence, current modelling practice where the settling behaviour only depends on a lumped variable such as concentration is insufficient to describe the true settling dynamics in WRRF processes.

Therefore, an extension of existing modelling frameworks is proposed, including different particle classes to represent the distribution in particle properties. The result is a unified framework which allows description of the true distributed settling behaviour over the entire concentration range from dilute suspensions, where discrete settling occurs (e.g. for PSTs, granular sludge and clarification in SSTs), to concentrated suspensions in which the sediment is described as a permanently networked, compressible porous layer (e.g. at high concentrations in the sludge blanket of SSTs or at the bottom of PSTs). Moreover, the proposed framework can be further augmented with reaction terms to describe the migration of particles between different classes in order to capture the effect of changes in operational and loading conditions on the sludge composition and the associated settling behaviour. Ultimately, this would allow introducing more rigour into the way settling tanks are modelled, potentially leading to improved operation and control in WRRFs.

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