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Review

Research advances and challenges in one-dimensional modeling of secondary settling Tanks – A critical review

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ABSTRACT

Sedimentation is one of the most important processes that determine the performance of the activated sludge process (ASP), and secondary settling tanks (SSTs) have been frequently investigated with the mathematical models for design and operation optimization. Nevertheless their performance is often far from satisfactory. The starting point of this paper is a review of the development of settling theory, focusing on batch settling and the development of flux theory, since they played an important role in the early stage of SST investigation. The second part is an explicit review of the established 1-D SST models, including the relevant physical law, various settling behaviors (hindered, transient, and compression settling), the constitutive functions, and their advantages and disadvantages. The third part is a discussion of numerical techniques required to solve the governing equation, which is usually a partial differential equation. Finally, the most important modeling challenges, such as settleability description, settling behavior understanding, are presented.

Contents

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1. Introduction

Biological secondary treatment processes are widely used in wastewater treatment plants to remove organic matter and reduce nutrients such as nitrogen and phosphorus. In most cases, efficient operation requires the biomass to be removed from the wastewater by sedimentation, filtration or other solids-liquid separation processes.

Several types of treatment processes can achieve solids-liquid separation, but secondary settling tanks (SSTs) are most commonly used. SSTs, also known as sedimentation basins or solids-liquid separators, use gravity to separate the biomass from the fluid, and have two similar but distinct functions: clarification and thickening. Clarification is the removal of finely dispersed solids from the liquid to produce a low turbidity effluent; Thickening is the process of increasing the sludge concentration in order for it to be recycled or disposed in less volume. In SSTs, the clarification process occurs in the upper zone while thickening occurs near the bottom. The result is an effluent from the top, low in suspended solids, and a second stream of settled, concentrated biomass from the bottom, suitable for recycling or disposal.

As one of the most important units in wastewater treatment process, the SST is often a “bottle neck,” limiting the capacity of the wastewater treatment process (Ekama et al., 1997; Ekama and Marais, 2002). The SST sizing must be combined with the bioreactor sizing to provide the minimum necessary conditions, such as the solids retention (SRT) or food-to-mass (F/M ratio) to meet design conditions, as well as maintaining a safety factor to handle shocks and upsets. If the SST does not produce a highly clarified effluent, or cannot thicken biomass to the required recycle concentration, excessive effluent solids will result, causing effluent permit violations and resultant loss biomass from the reactor. Therefore, two commonly used parameters: overflow rate and solids flux, have been developed for SST design and evaluation.

Since wastewater characteristics vary, such as temperature, flow rate and contaminant concentrations, traditional design procedures for SSTs tend to be more empirical and conservative by introducing averaged parameters with safety factors (Coe and Clevenger, 1916). Therefore SST performance can suffer unanticipated fluctuations, which may cause process control problems and increase the risks of failure. Stringent standards for effluent quality and the need for optimization of WWTP performance have made such variations in effluent quality undesirable, and have encouraged the use of dynamic controls for wastewater treatment process.

A mathematical modeling approach, where the bioreactor models are coupled with SST models, is encouraged in WWTP studies for overall process design and control optimization. Scientific knowledge on characterizing the biomass growth and contaminant removal is well-developed, whereas the various settling behaviors within the SST are still poorly understood, thus causing the difficulty in effluent quality prediction, biomass inventory estimation (Plósz et al., 2011). Great efforts have been made to rigorously predicting the SST performance. According to different practical application purposes, the modeling approaches can be divided into three main categories:

1. One-dimensional (1-D) dynamic model: 1-D model is based mostly on the flux theory and Kynch's assumption that the solids gravity settling velocity is only determined by the local sludge concentration. The hydraulic flow is simplified as downward/upward flow to simulate the recycling/effluent flow and satisfy the 1-D assumption.
2. Two-dimensional (2-D) hydraulic model: compared with 1-D models, 2-D models are developed using computational fluid dynamics (CFD) techniques. Therefore, instead of simplifying or omitting the hydraulic flow impact, 2-D models can incorporate hydrodynamics such as density currents, turbulence, and artifacts unfavorable SST geometry. Flocculation behavior can also be modeled, if coupled with a sub-flocculation model (Zhou and Mccorquodale, 1992a, b). A frequent application of 2-D models is to improve SST geometry design and optimize performance.
3. Three-dimensional (3-D) hydraulic model: the motivation of developing 3-D approaches is to understand non-symmetric features: for example the heat exchange caused by the varying temperatures and wind effects. Very detailed computation grids are now feasible in order to capture geometric features as small as several inches (Gong et al., 2011; Xanthos et al., 2011; Ramalingam et al., 2012). However, the high resolution grids also require strong computing capacity and power which may limit the 3-D models' practicability.

In current engineering practice, 1-D dynamic models are used to predict effluent and recycle solids concentration as well as the sludge blanket height in the SST. Although many 1-D SST models are available and some of them, especially the Takács model (Takács et al., 1991), have been widely utilized in engineering practice, the prediction of the sludge settling characteristics and concentration profiles in and out of a SST is still far from satisfactory, because of the using of empirical functions and unreliable numerical techniques

(Bürger et al., 2011, 2012; 2013; Li and Stenstrom, 2014b). Therefore, most commercial simulators equipped with these models may fail to provide globally reliable simulations under some conditions (Bürger et al., 2012), and further research is still needed to improve the performance of 1-D SST models.

The first goal of this paper is to review batch settling and flux theory, which played an important role in the earliest SST investigations. The second part focuses on 1-D SST modeling techniques. We divided most established 1-D SST models into two categories: mass conservation law model-based and mass-momentum conservation law model-based, according to their governing physical law. Different impact factors, for example convection transport, hydraulic dispersion, compression, are also discussed in this part, and the most frequently used empirical functions such as settling velocity function, drag coefficient function as well as compressive yield stress function are well documented. The third part focuses on the numerical techniques used to solve the governing partial differential equations (PDEs), which is essential for obtaining accurate solutions. Finally, we give a brief review of the modeling difficulties in the current 1-D SST modeling investigations, and they can be summarized as settleability description, data availability and measurement technique, high numerical accuracy with low computational cost, and settling behavior understanding.

2. Batch settling study and flux theory development

Because of the similarities between batch settling and continuous settling processes, many early researchers investigating activated sludge thickening and clarification predicted continuous settling behavior from batch settling tests. Coe and Clevenger (1916) provided one of the earliest examples relating batch settling phenomenon to the design and operation of the SST, and in their classical paper, the settling behavior in a batch thickening column was qualitatively indentified in four distinctive zones: 1) the clear supernatant zone at the top with low turbidity; 2) the uniform settling zone with constant concentration equal to initial concentration; 3) the transition zone between the constant concentration and compression zones, and 4) the compression zone formed by the compression from overlaying sludge and the mechanical support of the lower bottom. Among each zone in the batch settling test, the constant settling zone was found to govern the SST area requirement; however Coe and Clevenger (1916) believed that the SST depth, in their case of using pulp and paper sludge, should be large enough to provide sufficient storage time, thus making the sludge retention long enough within the SST to squeeze the water out of sludge sediment to obtain more condensed recycling flow. As an extension of this conclusion, the requirement of SST area was characterized as the finding the minimum solids handling capacity for any intervening values from the initial concentration to the bottom (Coe and Clevenger, 1916).

As the only established quantitative approach, Coe and Clevenger's empirical procedure was widely accepted and used in the first half of the 20th century, having a profound impact on SST design and operation. Nevertheless, the remaining difficulties of theoretically examining the settling process still prevented the in-depth understanding of the batch settling process, as well as the continuous process.

In order to simplify the problem without having to understand the detailed force acting on particles, Kynch (1952) presented the constitutive relation, now known as Kynch's assumption, that the hindered settling velocity is uniquely determined by the local solids concentration. On the basis of Kynch's assumption, the batch settling process was modeled by the mass continuity equation of the solid phase as eq. (1) with proper constitutive functions, initial and boundary conditions, and the mass flux was introduced for solids conveyance calculation:

$$\frac{\partial \phi}{\partial t} + \frac{\partial(\phi v_s)}{\partial z} = 0 \tag{1}$$

where ϕ is the solid concentration, v_s is the gravity settling velocity, t is time, z is the spatial axis in vertical direction.

In solving Eq. (1), solution discontinuities are expected to occur as a function of time and height, and these discontinuities can be physically interpreted as the sediment interfaces or blanket heights observed in experiments and full-scale operations. Therefore, Eq. (1) is satisfactory in capturing concentration discontinuities without knowing their physical mechanisms, although it fails to distinguish various settling behaviors (Kynch, 1952; Concha and Bürger, 2003). As Kynch said in his celebrated paper "a considerable amount can be learned by the single main velocity assumption, though further experiments are necessary to verify its validity" (Kynch, 1952). His theory greatly improved the understanding of the settling problem, and usually has been applied as the first step in batch and continuous settling data analysis.

Since the starting point of Kynch's work is a mathematic development and analysis of Eq. (1), he did not provide suggestions for practical application of his theory. The first attempt of introducing Kynch's theory to SST design was proposed by Talmage and Fitch (1955). In their design procedure, the slope of a tangent to the interface subsidence curve of a batch settling test was thought to be equal to the settling velocity of the layer with the initial concentration, shown as Fig.1, which is consistent with Kynch's theory. Therefore, the settling velocity information can be obtained through the initial and final equilibrium states, and the settling flux curve can be synthesized from a single batch settling test.

Shortly thereafter, Talmage and Fitch made the assumption that the thickening capacity is governed by the concentration which exists at the solid–liquid interface as the solids enter the compression zone. If solids enter the compression zone more rapidly that they can pass through it to the underflow, accumulation occurs. Hence, the accuracy of their design procedure is highly dependent on precisely determining the time of compression (t_c). Several empirical methods are available: Roberts' (1949) procedure based on Coe and Clevenger's hypothesis that the loss of water in the compression zone is a function of time and Eckenfelder and Melbinger's (1957) tangents crossing method.

In additional to the difficulty of determining the compression time, the Talmage-Fitch procedure subsequently

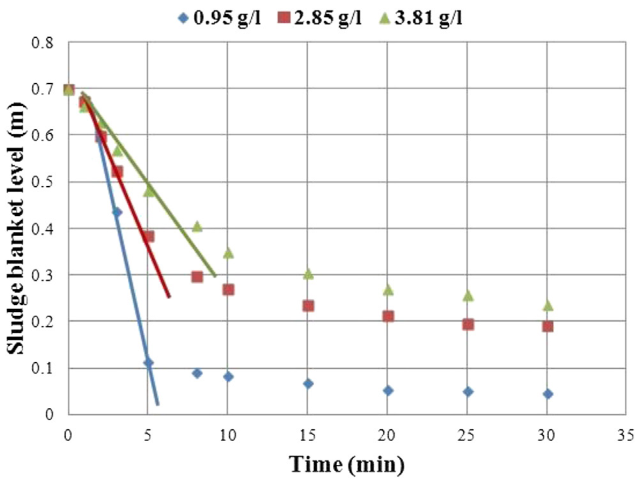

Fig. 1 – Sludge blanket height *vs.* time (Grieves and Stenstrom (1976)).

has been shown to yield conservative SST size design by many investigators (Hassett, 1958; Fitch, 1962; Alderton, 1963). One explanation for this result is that the settling velocity is not only determined by concentration in compression zone but also impacted by various other factors, such as the compressive force, which invalidates Kynch's original assumption. However, acknowledging its shortcomings, the Talmage-Fitch procedure was still advocated by a number of researchers, because it requires only one batch settling test, as opposed to multiple batch settling experiments required by the Coe and Clevenger method (Moncrieff, 1964; Scott, 1968a, b).

The reason the Talmage and Fitch method leads to a conservative design rests on two important assumptions: the first is that the settling velocities observed in laboratory batch settling test can truly represent those found in full scale SSTs, and the second is the validity of the Kynch assumption itself.

To understand the potential artifacts of small scale equipments, factors such as the cylinder size, the initial sludge height were investigated. When the diameter of the batch settling cylinder becomes fairly small with respect to the particle size, for example in 1 L graduate cylinder (diameter = 3 cm), the "wall effect" will be greatly magnified by "arching" or "bridging" of the sludge with the wall, which could retard the normal settling process (Kammermeyer, 1941; Vesilind, 1968). Dick (1965) showed that the "wall effect" was more profound with the concentrated sludge than with dilute one. Generally, the small diameter column can produce higher settling velocity in the dilute range, but lower velocities in the concentrated range (Vesilind, 1968). Small size cylinders are more convenient to use since they require less test sludge, and obtaining uniform initial sludge concentration throughout the cylinder is easier. Non-uniform sludge concentrations may invalid the 1-D assumption may also change floc characteristics (Tracy, 1973). For these reasons small size cylinders are still desirable, and slow speed mixers have been recommended to avoid wall effects (Work and Kohler, 1940; Behn, 1957), as well as model the rake effect found in full-scale SSTs (Eckenfelder and Melbinger, 1957; Vesilind, 1968).

Differences in observed settling velocities have been attributed to the initial depth of the sludge. Several researchers (Work and Kohler, 1940; Kammermeyer, 1941) showed that the initial settling depth exerts a profound influence in concentrated sludge experiments while having much less influence in dilute sludge experiments. Later, more detailed investigations from Dick and Ewing (1967) showed that the height effect was closely related to the type of sludge; for example activated sludge was much more influenced by initial depth than a suspension of sand. Shannon et al. (1964) used glass beads with a Gaussian size distribution to demonstrate the independence of settling velocity with the initial height, and Kynch's theory was applicable for interface height prediction (Shannon et al., 1963). This discrepancy was caused by the fact that the activated sludge deviates greatly from the ideal particle assumption (Tracy, 1973). The validity of Kynch's theory in compression zone was proven by Tory and Shannon (1965), and they stated that the settling velocity in compression zone can still largely be approximated as a function only of concentration.

The settling velocity function is significant for SST design using solid flux theory (Cho et al., 1993), and a variety of theoretical or empirical functions have been proposed (Steinour, 1944; Vand, 1948; Richardson and Zaki, 1954; Yoshioka et al., 1957; Scott, 1966; Vesilind, 1968; Vaerenbergh, 1980; Takács et al., 1991; Cho et al., 1993; Cacossa and Vaccari, 1994; Bürger, 2000; Kinnear, 2002; Zhang et al., 2006). Various factors, for example the particle size, shape, sludge viscosity, density and porosity have been used to characterize the settling velocity, while in practical engineering application, empirical functions are preferred due to their simplicity and practicality. For applications relating to municipal wastewater treatment, the most popular are the exponential functions (Vesilind, 1968; Takács et al., 1991), which have been shown to better fit the experimental data than other functions (Smollen and Ekama, 1984). Most empirical approaches primarily determine the hindered settling velocity as a function of the sludge concentration, although a few functions, consider the velocity in the compression zone, which deviates with Kynch's assumption, and will be discussed later.

The main difference in the continuous settling process as compared to batch settling, is the bulk solids transport caused by hydraulic flows, and in ideal 1-D conditions, these hydraulic flows are simplified as the upward and downward bulk flow, which convey the sludge towards the SST effluent weir and bottom, respectively. On the basis of considering the hydraulic bulk transportation, Yoshioka et al. (1957) and Hassett (1958) independently developed two widely used graphical methods for the limiting flux and SST operation condition analysis. The former one plots gravity flux only, while the later shows both gravity and total flux (total flux = gravity flux + bulk flux). The SST area requirement is governed by the local minimum flux point, which is therefore termed as the limiting flux, and the recycling solids concentration is estimated from mass conservation around the SST bottom. Scott (1968a, b) noted that since both methods were based on batch flux data, they might overestimate the limiting flux and recycling concentration, because batch settling tests do not included a deep compression zone required for compression.

Different batch settling materials or sludges, including the carbonate sludge, lime softening sludge and activated sludge have been used to verify limiting flux theory, and good agreement between observed thickening performance and prediction based on batch flux analytical methods were obtained in all cases (Yoshioka et al., 1957; Hassett, 1958; Javaheri, 1971). Thereafter, Keinath et al.(1977) and Keinath (1985) extended these methods to the state point concept, where the state point is the intersection of the recycle flow and overflow lines on the settling flux plot. State point analysis is now commonly used to evaluate SST performance over a range of different operating conditions (underloading condition, critical loading condition and overloading condition), as well as predicating the vertical concentration profiles.

Despite its prevalence, the solids flux theory still has two remaining problems: 1) it is an experiment observation result more than a theoretical proved conclusion; 2) it can deal with steady states, but fails in dynamically investigating the settling behavior within SSTs. During the 1990s, the development of 1-D SST model and mathematic techniques of nonlinear hyperbolic PDEs provide the opportunity of further understanding the solids flux theory. Chancelier et al. (1997) found that the flux theory can be confirmed and extended in a natural way within the context of the nonlinear hyperbolic PDEs, and the flux theory conclusions are closely related to the stationary solutions of the 1-D model governing equations. By describing the solids flux theory within nonlinear PDEs theory, many defined conceptions as the limiting flux, feed layer, sludge blanket height and loading condition can be interpreted by a first-order hyperbolic PDE model, hence making the SST dynamic behaviors predictable (Diehl, 1995, 1996; Bürger and Narvaez, 2007; Bürger and Karlsen, 2008; Diehl, 2008). Obviously, compared with the stationary solutions of the flux theory, the 1-D SST model owns the specific advantage in dynamic or transient conditions predictions, for example the shock hydraulic loading caused by rainfall, or the sludge bulking problem caused by filament growth. This explains why the research interests was changed to develop reliable 1-D SST model for more comprehensively quantitative investigation of SST design and operation, which will be discussed in the following section.

3. 1-D mathematical modeling of ssts

SSTs have been investigated with mathematical models for design and operation optimization purposes. Although several 2-D and 3-D SSTs models have been developed, 1-D models are mostly used because of their simplicity and lower computational demands. Before discussing 1-D SST models and their development, it is informative to define the expected capabilities of an acceptable model (Tracy, 1973). Firstly, the 1-D model should be able to predict both effluent and underflow concentrations during transient operating conditions, which corresponds to clarification and thickening processes. The second main function is to approximate the concentration profile and sludge blanket level during unsteady-state operating condition in order to avoid system failure. Moreover, the model should be able to integrate with available bioreactor models to provide an overall secondary treatment simulation for system design and operation optimization purposes.

Given the complexity of real system conditions (e.g., viscosity, dispersion, turbulence, rake effect, various settling behaviors) and the need to simply the model, several ad hoc assumptions are usually introduced to limit application to an ideal suspension (a continuum) and 1-D modeling conditions, as follows:

1). the SST is circular and central-feed with constant section area;
2).the reaction rates are zero in the SST, and the particle properties (not concentrations) are uniform and constant in the SST;
3). the hydraulic flows are vertically, and horizontally uniform (no density currents or wind effects) and the solids concentration are uniform across any horizontal cross-section of SSTs;
4). the mechanical sludge scraper does not impact the settling process and wall effects are negligible.

Based on these assumptions, Shannon et al. (1963) presented the concept of an ideal 1-D SST, and a number of later researchers have advanced these concepts (Bryant, 1972; Stenstrom, 1976; Bustos et al., 1990b; Bürger et al., 2011). Fig.2 shows the schematic overview of an ideal SST. In general, SSTs can be divided into three major zones according to their distinct functions: clarification zone, thickening zone and feed zone. In the clarification zone, influent flow is clarified to produce low turbidity effluent, while the thickening zone provides concentrated solids for recycling and disposal. The feed zone is the place where the input sludge is introduced and well mixed for initial settling. For 1-D modeling, the hydraulic flow divides and is upward flow (Q_e) towards the effluent weir and the downward flow (Q_u) towards the SST bottom. As can be seen, compared with the static sedimentation process in batch tests, the feeding and discharge flows in SSTs are continuous.

Instead of the sole gravity settling in batch settling tests, the hydraulic bulk transport caused by the upward and

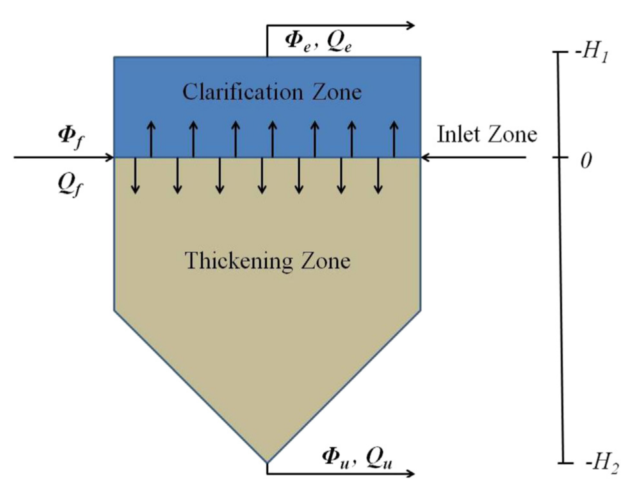

Fig. 2 – Schematic overview of an ideal one-dimensional SST.

downward hydraulic flows can also greatly impact the sludge settling behavior in the continuous settling process. Therefore, the combination of the sedimentation knowledge learned from batch settling tests and the concept of an ideal SST forms the fundamental theory framework of the 1-D SST modeling. The problem then becomes how to mathematically describe the continuous settling behavior based on this framework.

3.1. *The mass continuity model*

Generally, the starting point of mathematical modeling work is the physical law (Bürger et al., 2011). The mostly used one in 1-D SST modeling is the mass conservation law of the solid phase, which requires that the substance change per unit time in a finite region equals to the net flux into the region pluses the net mass production in the region, and usually the net mass production is negligible because of the zero reaction assumption. Using the ideal1-D assumptions, the solids concentration is a function of space (*z*) and time (*t*).

The mass conservation law model is also known as the layer model, which was originally presented by Bryant (1972) and Stenstrom (1976) for thickening process modeling, and broadened by Vitasovic (1986) by adding the layer above the inlet level for effluent flow quality prediction. The SST is divided into a fixed number of layers with uniform concentration in each layer, and the mass conservation law is imposed around each layer to generate the following nonlinear hyperbolic PDE formations (Takács et al., 1991; Diehl and Jeppsson, 1998; Diehl, 2000) by modeling the feed flux as point source:

$$\frac{\partial\phi}{\partial t}+\frac{\partial F(\phi)}{\partial z}=\upsilon_f\phi_f\delta(z)$$
$$F(\phi)=\begin{cases}-\upsilon_e\phi & \text{effluent zonek} \quad (z<-H_1)\\ \upsilon_s\phi-\upsilon_e\phi & \text{clarification zone} \quad (-H_1<z<0)\\ \upsilon_s\phi-\upsilon_e\phi+\upsilon_u\phi & \text{inlet zone} \quad (z=0)\\ \upsilon_s\phi+\upsilon_u\phi & \text{thickening zone} \quad (0<z<H_2)\\ \upsilon_u\phi & \text{underflow zone} \quad (z>H_2)\end{cases} \tag{2}$$

where H_1 is the height of the clarification zone, the feed point is located as $z=0$, H_2 is the depth of the thickening zone, see Fig.2; $\delta(z)$ is the Dirac impulse; υ_e is the effluent flow velocity, υ_u is the downward flow velocity, υ_f is the feed flow velocity, ϕ_f is the feed concentration. Compared with the batch settling governing equation (Eq. (1)), the continuous settling PDE framework includes two bulk terms ($\upsilon_e\phi$ and $\upsilon_u\phi$) to capture the hydraulic transport process. After adding suitable initial and boundary conditions, solving Eq. (2) is a problem with one equation and two unknowns. As in the batch settling modeling approach, the constitutive relation (Kynch's hindered settling velocity assumption) is again used to provide a unique solution. The validity of Kynch's concentration discontinuity theory in predicting sludge blanket level propagation in SST has also been demonstrated by solving Eq. (2) with reliable analytical or numerical techniques (Bustos et al., 1990a; Diehl, 1996, 2000; Bürger et al., 2003). Because of its success in hindered settling modeling, others (Fitch, 1983; Font, 1988) have added compression effect terms based on Kynch's theory. However, this kind of modification encountered several problems that are not easy to solve within Kynch's theory (Concha and Bürger, 2003), which will be discussed in the compression effect modeling section.

3.1.1. *Settling velocity determination*

The determination of the appropriate settling velocity function is essential in the 1-D SST modeling process (Cho et al., 1993). Though the settling velocity is physically a function of the particle and fluid properties, including the particle shape, size distribution, fluid and floc density, fluid viscosity and the hydrodynamic resistance, most available settling velocity models are still empirical with the model parameters determined by experimental curve fitting techniques, such as the single batch settling curve fitting method (Cacossa and Vaccari, 1994; Vanrolleghem et al., 1996).

The two mostly used settling functions are the power law function (Eq. (3)) and exponential law function (Eq. (4)):

$$\upsilon_s=k\phi^{-n} \tag{3}$$

$$\upsilon_s=k\exp(-n\phi) \tag{4}$$

The power function was first suggested by Yoshioka et al. (1957). However, the accuracy of the power law model deteriorates in dilute sludge region (below 2 kg m^{-3} (Pitman, 1980) or below 3 kg m^{-3} (Riddell et al., 1983)) and becomes infinite at zero concentration. This problem can be solved by two alternative approaches: artificially imposing a maximum velocity value or using another velocity function for the dilute concentration zone (De Clercq et al., 2008).

The exponential model is also known as the Vesilind model (Vesilind, 1968) that distinct from the power one in both the dilute and condensed zone prediction. It provides a reasonable maximum when the concentration approaches zero, and lower velocity in the high sludge concentration range compared with the power law model predictions. Smollen and Ekama (1984) also showed that the exponential model gave a better fit with the experimental data than the power model. Although the exponential model has special advantages over the power model, it is still fully empirical and the parameter values depend upon the fitting experimental data.

From a practical standpoint, Takács et al. (1991) questioned the validity of the exponential model in the dilute zone believing that the dilute zone settling velocity be impacted by the flocculation process and non-settleable solids fraction. They modified the exponential model to Eq. (5), now known as the Takács model, to account for these factors:

$$\upsilon_s=\max\left(0,\min\left(\upsilon_{0,\max},\upsilon_0\left(\exp^{-n_1(\phi-\phi_{\min})}-\exp^{-n_2(\phi-\phi_{\min})}\right)\right)\right) \tag{5}$$

The term (υ_0 $exp^{(-n_1\ (\phi-\phi))}{}_{\min}$) reflects the settling velocity of the large, well flocculated particles, while the term (υ_0 $exp^{(-n_2\ (\phi-\phi))}{}_{\min}$) is the velocity correction factor of the smaller slowly settling particles. $\phi_{\min}$ indicates the non-settable solids fraction. The Takács and Vesilind models only differ in the dilute sludge region, which impacts the predicted effluent TSS concentration.

There have also been efforts to derive the settling velocity from fundamental analyses of mass and force acting in the two phase flow (Cho et al., 1993; Cacossa and Vaccari, 1994; Kinnear, 2002). Starting from the Carman-Kozeny equation which is accepted universally for porous media modeling, Cho et al. (1993) deduced the settling velocity function by adding the sludge viscosity term. Eq. (6) uses the viscosity as an exponential function, Eq. (7) is valid when the sludge volume fraction is negligible of the total volumetric concentration (low sludge concentration) and Eq. (8) is the situation where the viscosity term is constant.

$$v_s = k(1-n_1\phi)^4\exp(-n_2\phi)/\phi \tag{6}$$

$$v_s = k\exp(-n\phi)/\phi \tag{7}$$

$$v_s = k(1-n\phi)^4\Big/\phi \tag{8}$$

Comparison of data and models showed that this model can perform well without causing the infinite problem in dilute range, and also can be easily used within the limit flux theory (Cho et al., 1993).

To complement the velocity model for compression zone calculation, Cacossa and Vaccari (1994) originally developed the model in terms of the total suspended solids concentration, the dynamic pressure gradient and the gradient corresponding to the compressive yield stress as shown in Eq. (9).

$$v_s = v_0(1-(\partial\phi/\partial z)/K) \tag{9}$$

where K is defined as the compressibility function, which describes the sludge compressive properties. As opposed to the Kynch assumption based models, the settling velocity in this model is defined as a function of the solids concentration, as well as gradient in solids concentration. The batch setting verification results showed that it may over predict the solid–liquid interface level in the compression region, and a more elaborate expression of the compressibility function (K) is required for more accurate prediction (Cacossa and Vaccari, 1994). Kinnear (2002) followed this suggestion, and provided an improved velocity model by using more fundamental properties parameters, such as the solids volumetric concentration (ε), intrinsic permeability (k), floc and liquid density (ρ_f and ρ_l), specific surface area of the primary particle (S_0), sludge viscosity (μ), gel concentration (ε_g) and effective compression stress (P_0). The model was developed from the mass and momentum continuity equations of two phase flow. The hydrodynamic interaction coefficient was related to the intrinsic permeability, which was calculated by the Carman-Kozeny equation. The effective solids stress was determined by Buscall and White's (1987) empirical function, thus making the final settling velocity formulation expressed as:

$$v_s = \frac{\left(\rho_f-\rho_l\right)g(1-\varepsilon)^3}{5S_0^2\varepsilon\mu} \quad \text{for } \varepsilon<\varepsilon_g \tag{10}$$

$$v_s = \frac{\left[\varepsilon\left(\rho_l-\rho_f\right)g + P_0\left(\frac{\varepsilon}{\varepsilon_g}\right)^m\frac{\partial(1-\varepsilon)}{\partial z}\right](1-\varepsilon)^3}{5S_0^2\varepsilon^2\,\mu} \quad \text{for } \varepsilon>\varepsilon_g \tag{11}$$

In contrast to the empirical models, Eqs. (10) and (11) incorporate the basic physical factors that may determine the sludge settleability, and their derivation does not rely on Kynch's assumption. Again, the settling velocity is function of both the solids concentration and concentration gradient as in the Cacossa-Vaccari model.

Most velocity functions discussed so far, and especially the power and exponential models, are only appropriate for hindered/compression region modeling, and extending these functions into the flocculation region can produce unrealistic results (Kinnear, 2002). Incorporating a more complex flocculation model, as in the Takács model, by introducing a term to reflect the settling velocity of large, well-flocculated particles, or simply setting a constant settling velocity that can be measured during pilot testing, which is the same strategy as used in the power model to limit the overprediction of the settling velocity in the dilute region.

Table .1 summarizes the structure of various settling velocity functions, and their proper modeling domains. To estimate the performance of these velocity functions, we provided a typical function calibration example, based on the full-scale data collected by Grieves and Stenstrom (1976) and Levenberg–Marquardt algorithm (More, 1978). Fig.3 shows the data fitting result. It is noticeable that almost all velocity models can fit the data in medium concentration range very well, but they deviate significantly in both dilute and high concentration conditions, which also has been demonstrated in previous studies.

3.1.2. *The Stenstrom flux constraint analysis*

The well-known flux constraint was originally suggested by Stenstrom (1976) to limit the mass flux for solids overloading simulation. Based on the assumption that the settling mass flux into the lower layer can never exceed the flux the layer is capable to transmit, the flux constraint can be expressed as Eq. (12).

$$F^S_{i+1/2} = \min\left(v_{s,i}\phi_i, v_{s,i+1}\phi_{i+1}\right) \tag{12}$$

where S is the Stenstrom numerical flux, i denotes the layer i. Although this flux limiting constraint is empirical, it is "consistent", which means the numerical flux should be a function related to adjacent layers instead of the local single layer (Bürger et al., 2011). By implementing this numerical flux constraint, Stenstrom's model was capable of capturing the sludge blanket change under various operating conditions, thus making the SST failure predictable. Bürger et al. (2011) showed that this constraint is indeed a specific numerical flux for unique solution calculation rather than a physically existing one, and noted it as the Stenstrom flux. However, this flux constraint is not nostrum, and will cause unphysical solution oscillations under several conditions such as in the negative concentration gradient case. A site specific threshold concentration was recommended to be set below which the constraint is inactive (Vitasovic, 1986; Takács et al., 1991). The best well-known work following the Stenstrom flux constraint is the Takács' 10-layer model (Takács et al., 1991), which has been mostly used in WWTP modeling.

Watts et al. (1996) tested the Takács model in various discretization levels (10, 20, 50 layers) without changing the model parameters, and found that only 10-layer provided good agreement with Pflanz's data (Pflanz, 1969). Increasing the number of layer will considerably deteriorate the model

Table 1 – Overview and comments of gravity settling velocity functions.

Model type	Model formula	Source	Comments
Polynomial models	$v_s = k(1 + n_1\phi + n_2\phi^2 + n_3\phi^3 + n_4\phi^4)$	Shannon et al. (1963)	≻empirical model; ≻not often used in practical engineering application; ≻provides unreliable approximation in low concentration range ≻requires more parameters than other models;
	$v_s = k\phi(1-\phi)$	Scott (1966)	
	$v_s = \sqrt{n_1/(n_2 + n_3\phi + n_4\phi^2 + n_5\phi^3)}$	Stenstrom (1976)	
Power models	$v_s = k(1 - n\phi)^{4.65}$	Richardson and Zaki (1954)	≻empirical model; ≻often used in practical engineering application; ≻overestimate settling velocity when concentration is small; ≻singular when concentration approaches to 0;
	$v_s = k\phi^{-n}$	Yoshioka et al. (1957)	
	$v_s = k(1 - n_1\phi)^{n_2}/\phi$	Scott (1966), Cho et al. (1993)	
	$v_s = k(1 - n_1\phi)^{n_2}; v_s = k_1(1 - n_1\phi)^{n_2} + k_2$	Vaerenbergh (1980)	
Exponential models	$v_s = k(1 - n_1\phi)^2 \exp(-n_2\phi)$	Steinour (1944)	≻empirical model; ≻often used in practical engineering application; ≻provide reasonable velocity estimation in all concentration domains; ≻includes other effects, such as flocculation settling, non-settleable particle fraction;
	$v_s = k(1 - n_1\phi)^2 \exp(-n_2\phi/(1 - n_3\phi))$	Vand (1948)	
	$v_s = k \exp(-n\phi)$	Vesilind (1968)	
	$v_s = \max(0, \min(v_{0,\max}, v_0(\exp^{-n_1(\phi-\phi_{\min})} - \exp^{-n_2(\phi-\phi_{\min})})))$	Takács et al. (1991)	
	$v_s = k \exp(-n\phi)/\phi; v_s = k(1 - n_1\phi)^{n_2} \exp(-n_3\phi)/\phi$	Cho et al. (1993)	
Compression effect including models	$v_s = v_m(1 - (\partial\phi/\partial z)/K)\begin{cases} v_m = (2 - \phi/\phi_g)(n_1/(\phi_g - n_2)) & \text{if } \phi < \phi_g \\ v_m = (n_1/(\phi_g - n_2)) & \text{if } \phi \geq \phi_g \end{cases}$	Cacossa and Vaccari (1994)	≻semi-empirical model derived from mass and momentum conservation law; ≻often used in compression settling behavior studies; ≻most parameters have physical meaning, and can be estimated by experiment measurements instead of curve fit;
	$v_s = v_{hs}(\varepsilon) \text{ if } \varepsilon < \varepsilon_g; v_s = v_{hs}(\varepsilon)\left(1 - \frac{\rho_s \sigma_e'(\varepsilon)}{\varepsilon_g \Delta\rho} \frac{\partial\varepsilon}{\partial z}\right) \text{ if } \varepsilon \geq \varepsilon_g$	Bürger et al. (2000)	
	$v_s = \frac{(\rho_l - \rho_s)g(1-\varepsilon)^3}{5S_0^2\varepsilon\mu} \text{ if } \varepsilon < \varepsilon_g; v_s = \frac{(\varepsilon(\rho_l - \rho_s)g + \sigma_e'(\varepsilon)\partial(1-\varepsilon)/\partial z)}{5S_0^2\varepsilon\mu}(1-\varepsilon)^3 \text{ if } \varepsilon \geq \varepsilon_g$	Kinnear (2002)	

performance, which is contradictory to the fundamental principle that the finer discretization should provide more accurate predictions. Further investigation of the Stenstrom flux constraint implied that the function of the flux constraint equals to a layer thickness dependent dispersion term, and its function disappears as the layer thickness approaches to zero, which explains the Takács model deterioration with the increasing discretization level (Watts et al., 1996). To correct this problem, Watts et al. (1996) added a dispersion term, hence improving its fit to the Pflanz in finer discretization condition.

Despite analyzing the Stenstrom flux constraint physically, the studies from the standpoint of numerical techniques demonstrated that the inclusion of the Stenstrom flux constraint is correct in the way of preventing the creation of shock wave and any inverse gradients in the concentration profile (Jeppsson and Diehl, 1996; De Clercq, 2006; Bürger et al., 2011,,2012; 2013). However, the model integrated with the Stenstrom flux constraint, such as the Takács model, can only fit the experiment data well in 10-layer condition, which is insufficient to resolve the detailed behavior of SSTs, and at least 30-layer is recommended for reliable predictions (Jeppsson and Diehl, 1996). To uniquely determine the reliable solution, both the 'consistent' principle and entropy condition which analogous to the second law of thermodynamic should be fulfilled (Bürger et al., 2011). The Stenstrom flux constraint satisfies the 'consistent' principle, but not always takes the entropy condition into account, which in return results unphysical solutions (oscillation) (Bürger et al., 2011, 2012; 2013). Bürger et al. (2013) suggested the approach of upgrading the Stenstrom flux constraint to the reliable Godunov flux, since they have similar mathematical expressions. As a conclusion, although the application of the Stenstrom flux constraint in 1-D SST modeling has achieved some degree of success, more fundamental numerical techniques are still encouraged to being introduced for entire reliable solution solving (for detailed information, see the numerical technique section).

3.1.3. *The convection-dispersion model development*

The success of the Kynch's theory in settling behavior analysis provided a firm foundation for the development of 1-D SST modeling studies. The mathematical discontinuities predicted by the Kynch theory, however, cannot exist in a practical system (Fitch, 1993), which has been confirmed by various experiment cases with continuous concentration profiles (Pflanz, 1969; Anderson, 1981; Bergstrom et al., 1992; Kinnear, 2002). A parabolic second-order PDE can provide a continuous or smooth concentration profile, and inclusion of an eddy turbulent diffusion term in the first-order hyperbolic PDE (Eq. (2)) converts the governing PDE to a parabolic one (Anderson, 1981; Vitasovic, 1986). This approach was implemented by Hamilton et al. (1992) and modified by Lee et al. (1999) with constant dispersion coefficients as Eq. (13) shows, and this model is capable of providing non-uniform, monotonically increasing concentration profiles with depth as expected.

$$\frac{\partial\phi}{\partial t} + \frac{\partial F(\phi)}{\partial z} - D\frac{\partial^2\phi}{\partial z^2} = v_f\phi_f\delta(z) \tag{13}$$

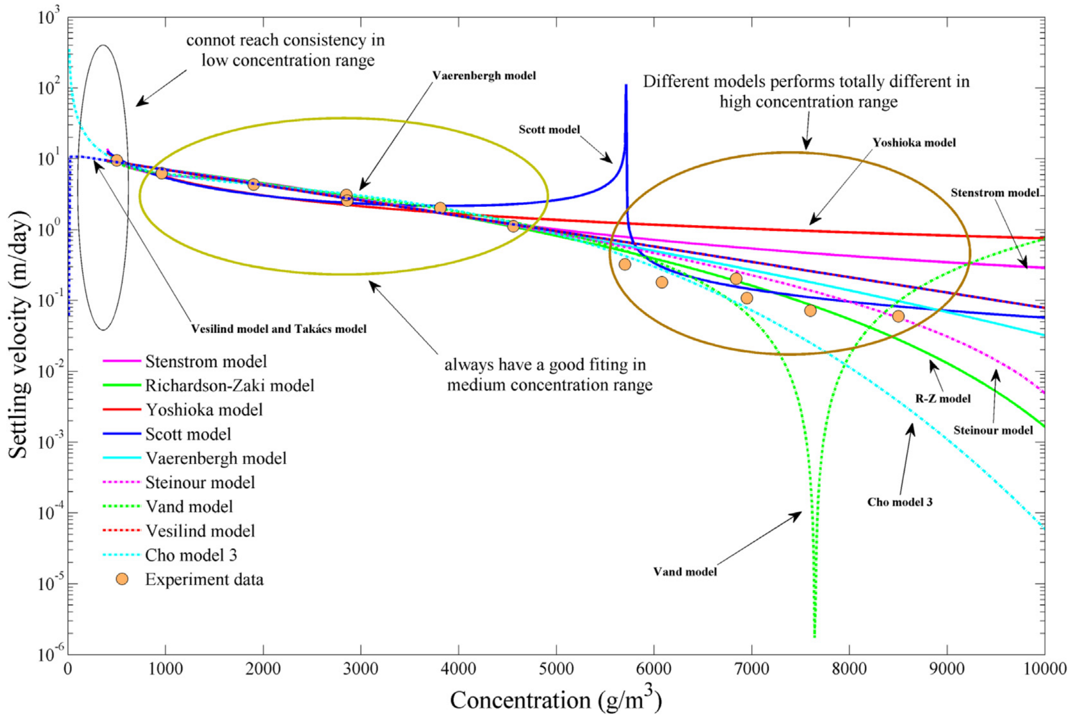

Fig. 3 – The fit of various settling velocity functions to the data collected by Grieves and Stenstrom (1976).

where D is the dispersion coefficient as a constant for the overall SST domain. Grijspeerdt et al. (1995) compared several established 1-D SST models and found Hamilton's and Takács's models are more reliable for fitting data because of their dispersion characteristics, even though the Takács model does not include a physical dispersion term. This can be explained by Watts' conclusion that in low discretization level, the function of the Stenstrom flux constraint equals to a layer thickness dependent dispersion term (Watts et al., 1996). Takács (2008) further demonstrated that in "rough" discretization condition, such as 10-layer, imposing the Stenstrom flux constraint introduces significant numerical dispassion that effective in smooth concentration profile developing. Nevertheless, the drawback of this smooth profile finding approach is the lack of control over the dispersion effect to best model calibration of various operating conditions (Plósz et al., 2011). A finer discretization, when the layer thickness approaches to zero, can seriously deteriorate the Takács model performance, since the dispersion function vanishes; discretization of 10-layers for the Takács generally approximates the dispersion expected in an SST.

To correct this problem, a modification of the concentration dependent dispersion coefficient is necessary, and one approach is to incorporate a dispersion coefficient that is a function of the hydrodynamic dispersion phenomenon caused by the turbulent currents. Even though the dispersion term is analogous with the Fick's constitutive relation for particle diffusion, it represents the hydrodynamic dispersion phenomenon caused by the turbulence rather than the thermal diffusion process (Anderson, 1981; Bürger et al., 2011). Watts et al. (1996) determined the dispersion coefficient as a function of the feed flow velocity which creates mixing in the inlet region, where most energy dissipation and turbulence occur. The dispersion term was also expected to approximate the processes that affect the sludge settling other than the bulk convection and gravity settling (De Clercq et al., 2003). De Clercq et al. (2003) proposed that since the flow conditions may differ in the clarification zone and the thickening zone, the dispersion term should not be only governed by the feed hydraulic flow, but both the upward and downward bulk flow:

$$\begin{aligned} D_1 &= D_{11} e^{\alpha \frac{Q_e(t)}{Q_f(t)}} \quad \text{Clarification Zone} \\ D_2 &= D_{22} e^{\beta \frac{Q_u(t)}{Q_f(t)}} \quad \text{Thickening Zone} \end{aligned} \tag{14}$$

where D_{11}, D_{22}, α and β are dispersion parameters that need to be calibrated.

Plósz et al. (2007) investigated the factors that degrade 1-D SST model performance by incorporating the dispersion in terms for both the effluent solids concentration and the sludge blanket height, and found that though the dispersion model can account for the SST hydrodynamic flow effect on the thickening process, the clarification efficiency is limited by flow boundary conditions. The model was optimized to enhance clarification prediction by introducing a hydraulic dispersion term as a function of the upward flow velocity-dependent term. In most recent studies, the mixing currents were assumed to occur in certain locations, such as the SST inlet region, and the dispersion coefficient forms were highly dependent on location. For example, the dispersion term in the SST inlet region is a function of the hydraulic feed flow velocity (Bürger et al., 2011,,2012; 2013), and influenced by factors in other regions of the SST. The recent global parameter sensitivity analysis of the whole WWTP modeling shows that selecting of 1-D SST model, convection dominant (first-order) or convection-dispersion (second-order) models, not only impacts the SST behavior prediction, but also greatly influences the parameter selection and the calibration procedure of the WWTP models (Ramin et al., 2014).

Table 2 summarizes of currently available hydraulic dispersion functions. Despite the convection and dispersion effect modeling, the mass conservation law SST model can also involve some other impact factors, for example the current density can be accounted for by adjusting the inlet height according to the feed sludge concentration (Dupont and Dahl, 1995), but the maximum of the inlet height should be restricted to 53% of the SST depth (Plósz et al., 2007). For short-circuit simulation, a short-circuit factor Ω was introduced, which is a dilution factor that can be found by a simple mass balance over the SST, when the flow and concentration of influent and return sludge flow are measured, as well as the concentration at the bottom of the SST (Dupont and Dahl, 1995).

3.2. *The mass-momentum conservation law model*

As can be seen from the above discussion, the cornerstone of the mass continuity model is Kynch's assumption that the settling velocity of a particle depends only on the local solids concentration. Its validly, however, can only be proved in the zone settling region (Dixon, 1977a), even Kynch himself admitted in his celebrated paper that "until the details of the forces on the particles can be specified, it is impossible to state when our hypothesis is valid, even for a dispersion of identical particles." (Kynch, 1952). This uncertainty gives rise to some important controversies, such as the determination of SST capacity, and compression settling behavior modeling.

By taking into account of force action during thickening process, Dixon (1977a, b, 1978) showed that there is no flux limitation associated with the hindered zone because of the absence of necessary retarding forces, which contradicts the previous conclusion that the hindered settling zone determines the SST thickening capacity as the increase of the compression zone height can compact the sludge by squeezing water out of the sludge structure which then can accelerate the sludge conveyance in this zone (Coe and Clevenger, 1916; Kynch, 1952; Fitch, 1962). For most real settling materials, in particular, these well flocculated slurries such as activated sludge, they form compressible sediment layers which are characterized by curved iso-concentration lines rather than the straight characteristics predicted by the Kynch model (Bürger, 2000; De Clercq et al., 2008). Therefore, the mass continuity model based on the Kynch assumption is not sufficient for various type sedimentation problems, and the investigation of the mass-momentum conservation law model with a detailed force balance is necessary to provide a more complete understanding of continuous settling behavior, especially in the compression zone where the Kynch's assumption may not apply.

Generally, given the complexity of the two-phase flow problem, two points of view have been developed for problem analysis and governing equation deviation (Zuber, 1964):

1). Internal flow approach: the flow of the fluidized system is considered as a flow through a porous medium with

Table 2 – Overview and comments of different hydraulic dispersion functions.

Model type	Model formula	Source	Comments
Hydraulic dispersion function[a]			
Fickian dispersion term	$D_{(z,t)} = \text{constan } t\ (13\ \text{m}^2/\text{day})$ $D_{(\text{clarification zone},t)} = \text{constan } t_1; D_{(\text{thickening zone},t)} = \text{constan } t_2$	Hamilton et al. (1992) Lee et al. (1999)	>cannot properly characterize the dispersion effect caused by the hydraulic turbulence but not the molecular diffusion; >greatly decrease the complexity of numerically difficulty in solving the governing PDE;
Function of hydraulic bulk flow rate	$\begin{cases} D_{i,i+1} = D_{\max}\left(1+\beta\left(\sqrt{C_iC_{i+1}}-C_{crit}\right)\exp^{-\beta\left(\sqrt{C_iC_{i+1}}-C_{crit}\right)}\right) & \text{if } \sqrt{C_iC_{i+1}} > C_{crit} \\ D_{i,i+1} = D_{\max} & \text{if } \sqrt{C_iC_{i+1}} \le C_{crit} \end{cases}$	Watts et al. (1996)	>empirical model; >properly indicate the hydraulic dispersion effect caused by the hydraulic bulk flow;
	$D_{(\text{clarification zone},t)} = D_{11}\exp^{\alpha}Q_e/Q_f$; $D_{(\text{clarification zone},t)} = D_{22}\exp^{\beta}Q_u/Q_f$;	De Clercq et al. (2003)	>parameters determination depends on concentration profile fit;
	$D_C = D_{C,0}$ if $v_{ov} < v_{ov,C}$; $D_C = D_{C,0} + \gamma(v_{ov} - v_{ov,C})$ if $v_{ov} \ge v_{ov,C}$	Plósz et al. (2007)	>often imposed around the SST inlet zone to simulate energy dispassion;

[a] Numerical dispersion or dissipation introduced by the numerical methods is discussed separately.

limited permeability, and solid–liquid relative movement could be modeled by Darcy's law through porous media (Shirato et al., 1970; Kos, 1977; Cho et al., 1993; Fitch, 1993; Diplas and Papanicolaou, 1997; Holdich and Butt, 1997; Zheng and Bagley, 1998; Karl and Wells, 1999).

2). External flow approach: the hydraulic flow is considered as the external flow around a particle located in the suspension. The well-known Stokes settling velocity is modified for hindered settling velocity calculation, and the compression process is characterized by semi-empirical equations stemmed from the rheology studies (Zuber, 1964; Buscall and White, 1987; Auzerais et al., 1988, 1990; Buscall, 1990; Bürger, 2000; Bürger et al., 2000a; Kinnear, 2002; Usher and Scales, 2005; De Clercq, 2006; Usher et al., 2006; Grassia et al., 2011).

3.2.1. *Force action analysis and model development*

The fundamental basis of a mass-momentum law based model is the identification of the specific forces acting on the particles, but it is also the most difficult step. Benefiting from the last half century's developments in fluid dynamics and rheology analysis techniques, the detailed sedimentation information, such as the fundamental force analysis, particle interaction in different density ranges now is detectable, and provide new 1-D SST modeling approaches.

As discussed above, the batch settling process can be described as four various concentration zones within the a settling suspension: the clear supernatant zone, the hindered settling zone, the transient zone, as well as the compression zone (Coe and Clevenger, 1916). The totally different settling behaviors within these zones necessitate the imposition of force action analysis separately rather than investigating them as a whole. The force acting analysis for the supernatant zone, compared with the other three, is much more straightforward. The gravity, the buoyancy, and the drag forces are the three dominant forces, and their calculation follows the classical approaches. A stochastic Brownian force also exists, but it is negligible due to the large Peclet number.

Before introducing the hindered settling analysis, it is useful to review the definition of hindered settling: when hindered settling occurs, the contacting particles tend to settle as a zone or "blanket", maintaining the same relative position with respect to each other (Metcalf&Eddy, 2002). The two distinctive characterizations of hindered settling are the absence of direct particle–particle interaction and uniform concentration profile, such as the uniform initial concentration zone in batch settling. Since there is no direct particle–particle interaction and the settling particles remain relatively stationary to the neighboring ones, only the equilibrium between drag and gravity forces limits settling velocity (Dixon, 1977a). The increased concentration in the hindered settling region creates a hydrodynamic interaction between particles, and settling velocity no longer conforms to Stokes settling behavior as it did in the supernatant clear zone (Buscall and White, 1987; Buscall, 1990; Landman and White, 1992; de Kretser et al., 2003). This hydrodynamic interaction mainly impacts the hydrodynamic drag coefficient, which can be multiplied by a hindered settling factor, $R(\phi)$, to quantify the inter-phase drag effect (for detailed information, see the drag coefficient determination section).

Few studies refer to the transient zone, since it is not always observable in batch or continuous settling tests (Coe and Clevenger, 1916; Dixon, 1977a). The existence of this region is usually viewed as a smooth transition between the zone and compression settling regions, and the settling behavior in this region is usually physically unstable: the settling plots frequently provide inconsistent results (Shirato et al., 1970). In most conditions, the transient zone is characterized by a gradually increasing concentration gradient, and is described by Fitch's concentration gradient study (Fitch, 1993). As Fitch stated, a positive concentration gradient leads to a reduced settling velocity due to the dominant solids pressure gradient. Though Kynch's theory succeeds in predicting a concentration gradient, the settling velocity within a region of large concentration gradient is determined not as the hindered settling velocity, but a transition velocity, caused by retarding phenomenon associated with the concentration gradient. When the solids pressure gradient is positive, the suspension is mathematically "in compression", and four kinds of solids compression force can be physically identified: elastic, static, osmotic and dynamic (Fitch, 1993):

Elastic compression force is caused by the random motion and collisions of particles (thermal diffusion), which can be modeling by adding a diffusion term ($D\delta\phi/\delta z$). However, even though existence of this force can be proven, its magnitude compared with the gravitational force and hydrodynamic drag force is much smaller, thereby making it insignificant in retarding the settling process.

Static compression force is also known as the compressive yield stress and arises when a continuous network is formed within strong inter-particle interactions (de Kretser et al., 2003). This stress can be transmitted directly throughout the network, and the settling process, if this stress occurs, will be irreversibly retarded (Buscall, 1990). However, the static compression force only occurs above the gel point (the point where interparticle force results in a self supported network), while the transient zone concentration is expected at concentrations no greater than the gel point. Hence, the retarding phenomenon within the transient zone cannot be completely defined by static compression force theory.

Osmotic compression force occurs when the concentration spatially varies, such as a monotonically varying concentration, and the suspension is in a non-equilibrium state (Auzerais et al., 1988). The origin of this force can be illustrated as the force both particles and fluid molecules experience in proportion to the gradients of their respective chemical potentials (Batchelor, 1976). The colloidal solids within the well-flocculated suspension, however, only constitute a relatively small fraction of the total weight, hence their contributed osmotic press could be indeed insufficient to retard the settling behavior (Fitch, 1993).

Dynamic compression force is characterized as the force that causes the particle deceleration as it approaches the discontinuity or settles within a region having a concentration gradient, such as the transient zone (Dixon, 1977a, b, 1978; 1981). It originates from the excess local pressure required to squeeze fluid out interstitial floc areas to make them more concentrated (Fitch, 1993). The mathematical formulation of this force still has not been well defined, and the difficulty of including it in the governing equation prevents the further investigation of its impact to the settling process.

The formation of the transient settling zone is the result of one or more retarding forces, and further studies are still needed to indentify the mechanism of their contribution to the retardation process.

The study of compression effects is significant for applications as diverse as filtration and centrifugation of suspensions in the mineral industries, or sludge dewatering in wastewater treatment process to reduce the final disposed sludge volume (de Kretser et al., 2003). Dixon (1977a) stressed the importance of compression effect as having a critical role in sludge settling retardation which he associated with determining SST solids handling capacity. The existence of compression zones has been confirmed by many studies, and the terminology "compression settling" can be interpreted from different perspectives. For instance, Fitch (1993) stated that the suspension is in a mathematical compression condition when the pressure gradient term is positive. In more recent studies, from the view of "compressive rheology", the compression settling zone is defined as the zone with particle concentration over the gel point, and also characterized by the strong compressive yield stress transmitted in this zone (Buscall et al., 1987; Buscall and White, 1987; Buscall, 1990; de Kretser et al., 2003; Usher and Scales, 2005; Usher et al., 2006).

The study of compression effects date back to the 1920s when Terzaghi (1925) originally developed the consolidation theory in the field of solid mechanics. This theory was then applied by Behn (1957) for the settling of compressive slurries because of its mathematical analogy independent of magnitude of the stress gradients. The compression behavior of flocculated particles (Kaolinite) were firstly addressed by Michaels and Bolger (1962b), and the compression settling was assumed to be governed by gravitational force (gravity and buoyancy), hydrodynamic drag force and the stresses transmitted throughout the condensed network. Shirato et al. (1970) stated that the compression-permeability (C–P) cell method (Ruth, 1946; Grace, 1953; Tiller and Shirato, 1964) widely used for internal flow analysis, can lead to substantial errors from wall effects in batch settling tests, and used zinc oxide and ferric oxide floc data to determine sediment compressibility and permeability. The numerical solutions of higher concentration conditions were solved, and showed a favorable agreement with experimental results (Shirato et al., 1970). For shock (concentration discontinuity) investigation purposes, Auzerais et al. (1988, 1990) started their work with a comprehensive analysis of all forces active in both liquid and solid phases, including the gravitational force, inertial force, viscous, and interparticle stresses.

Most of the investigators discussed above emphasized the critical role that compressive pressure plays in compression settling. The origin of this stress and how to quantify it to determine the sediment compressibility still remain unclear. In the view of compression rheology, for sedimentation at high concentrations, direct particle interaction allows energy to be stored elastically within the particle network. The accumulation of these solids close to the cylinder bottom causes a concentration gradient, and adding the compression stress arising from the accumulated, unbuoyed weight of the particles to the force balance, accounts for this phenomenon (Buscall and White, 1987; Buscall, 1990). For colloidally-stable suspension or a well-flocculated suspension below the gel point, this stress is only the osmotic pressure, while for concentrations greater than the gel point, the stress is elastic, which is characterized as the physically measurable network strength: the compressive yield stress (Buscall et al., 1987; Buscall and White, 1987; Buscall, 1990; de Kretser et al., 2003).

Meanwhile, several parallel theories starting from geotechnical approaches (Terzaghi and Peck, 1948; Bürger et al., 1999, Bürger et al. 2000a; Garrido et al., 2000; Bürger et al., 2001) and filtration research (Tiller and Shirato, 1964; Tiller and Yeh, 1987; Lee et al., 2000) also made important contributions to the understanding of compression settling behavior using the effective solids stress (σ) and the solids pressure (p_s) to quantify the sediment compressibility. However, compared with the compression rheology approach of defining the compressive yield stress as an intrinsic 'material property', both the effective solids stress and pressure, in most cases, are defined as volumetric concentration dependent functions, thereby making them numerically equivalent to the compressive yield stress. Except for the significant conceptual difference, these compressibility quantifying approaches have the a similar rheological basis, and the relationship between volumetric concentration and the compressive stress (the effective solids stress, the solids stress and compressive yield stress) need to be defined for parameter estimation (de Kretser et al., 2003).

As a conclusion, with a comprehensive force action analysis of various settling zones, the five forces (gravity, buoyancy, liquid pressure, hydrodynamic drag force, and compressive yield stress) acting on a floc-phase control volume in 1-D condition can be explicitly shown in Fig.4 with proper force directions. The gravity and buoyancy forces can be expressed as a net gravitational force and the hydrodynamic drag force originates from particle-liquid relative motivation. The osmotic pressure arises from the spatial concentration variation while the compressive yield stress only exists above the gel point where a self-supported network is formed. Therefore, a typical batch settling process can be modeled using the following four governing equations: liquid and solid continuity equations (Eq. (15) and Eq. (16)), liquid and solid momentum continuity equation (Eq. (17) and Eq. (18)):

Liquid continuity equation.

$$\frac{\partial(1-\varepsilon)}{\partial t}+\frac{\partial((1-\varepsilon)v_l)}{\partial z}=0 \tag{15}$$

Solid continuity equation.

$$\frac{\partial(\varepsilon)}{\partial t}+\frac{\partial(\varepsilon v_s)}{\partial z}=0 \tag{16}$$

Liquid momentum equation.

$$(1-\varepsilon)\rho_l\frac{\partial v_l}{\partial z}+(1-\varepsilon)\rho_l v_l\frac{\partial v_l}{\partial z}=-(1-\varepsilon)\rho_l g-(1-\varepsilon)\gamma(v_l-v_s)-(1-\varepsilon)\frac{\partial p}{\partial z} \tag{17}$$

Solid momentum equation.

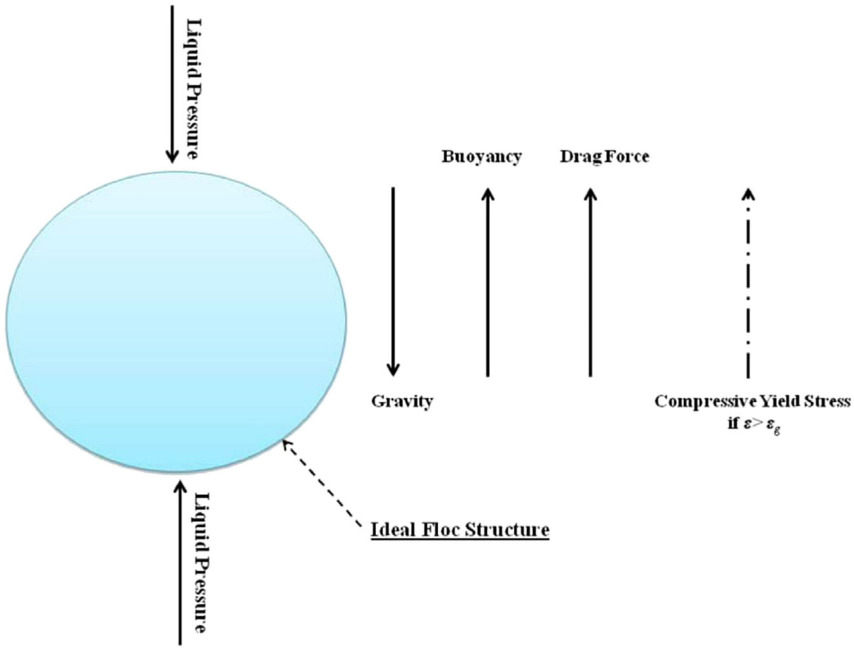

Fig. 4 – Force acting analysis of ideal floc structure.

$$\varepsilon\rho_s\frac{\partial v_s}{\partial z}+\varepsilon\rho_s v_s\frac{\partial v_s}{\partial z}=-\varepsilon\rho_s g+(1-\varepsilon)\gamma(v_l-v_s)-\varepsilon\frac{\partial p}{\partial z}\quad \varepsilon<\varepsilon_g$$
$$\varepsilon\rho_s\frac{\partial v_s}{\partial z}+\varepsilon\rho_s v_s\frac{\partial v_s}{\partial z}=-\varepsilon\rho_s g+(1-\varepsilon)\gamma(v_l-v_s)-\varepsilon\frac{\partial p}{\partial z}-\frac{\partial p_y}{\partial z}\quad \varepsilon>\varepsilon_g \tag{18}$$

where ε is the solids volumetric friction; ρ_l and ρ_s are the liquid and solid density; v_l and v_s are the liquid and solid velocity; g is the gravity acceleration; γ is the hydrodynamic drag coefficient; p is the fluid static pressure; p_y is the compressive yield stress;

The inertial term is always thought to be negligible, since it is many orders of magnitude less than the other terms (Auzerais et al., 1988; Karl and Wells, 1999; Bürger, 2000; Kinnear, 2002). Hence, the four governing equations can be simplified as the following equation:

$$\frac{\partial\varepsilon}{\partial t}+\frac{\partial}{\partial z}\left(\varepsilon\left(\left(\varepsilon(\varepsilon-1)(\rho_s-\rho_l)g+(\varepsilon-1)\frac{\partial p_y}{\partial z}\right)\Big/\gamma\right)\right)=0 \tag{19}$$

where$p_y=0$ if $\varepsilon<\varepsilon_g$, and $p_y>0$ if $\varepsilon>\varepsilon_g$. According to Dixon et al. (1976), the inertial term cannot always be ignored in sedimentation analysis due to its great significance in the interface between suspension and sedimentation where rapid velocity occurs. Fitch (1993) further stated that in the concentration gradient-occurring region, for example a transition settling region, various forces, including the inertial force, together with the dynamic pressure, osmotic pressure, and static pressure will be present, and if their resultant is negative, the inertial model is applicable due to the velocity augmentation of the inertial force. Therefore, compared with the simplification model (Eq. (19)), the original model (Eq. (15)–(18)) is more capable of describing an interface discontinuity, which is especially important for the sludge blanket level estimation in 1-D SST model. Obviously, additional proper constitutive functions are needed for the hydrodynamic drag coefficient and the compressive yield stress determination to make the model solvable.

3.2.2. *Hydrodynamic drag coefficient estimation*

Accurate calculation of the hydrodynamic drag force is especially important to describe hindered settling, since it is the only retarding force that can balance the positive gravitational force (Dixon, 1977a). At sufficiently low Reynolds number, the hydrodynamic drag force is proportional to the liquid–solid relative velocity, and can be expressed as Eq. (20):

$$F_d=\gamma(v_l-v_s) \tag{20}$$

Notice that v_l and v_s are the solutions of Eq. (17) and Eq. (18). Therefore, calculating the hydrodynamic drag force is equivalent to determining the hydrodynamic drag coefficient. Although various methods and constitutive functions have been developed for the drag coefficient estimation, most of them can be classified in three categories: the hindered settling factor approach (Richardson and Zaki, 1954; Michaels and Bolger, 1962b, a; Batchelo, 1972; Batchelor, 1976; Dixon et al., 1976; Buscall and White, 1987; Auzerais et al., 1990; Buscall, 1990; Landman and White, 1992; Chen et al., 1996; de Kretser et al., 2003; Usher and Scales, 2005; Usher et al., 2006), the Darcy's Law approach (Steinour, 1944; Javaheri and Dick, 1969; Davies et al., 1976; Cho et al., 1993; Islam and Karamisheva, 1998; Zheng and Bagley, 1998; Karl and Wells, 1999; Kinnear, 2002) and the Kynch batch flux density approach (Bürger, 2000; Bürger et al., 2000a, 2005; De Clercq et al., 2008; Bürger et al., 2011).

At a finite dilution with unbounded fluid, the hydrodynamic drag coefficient is the Stokes drag coefficient (λ_{st}); for instance, 6π for spheres, and the particle motion is balanced by the hydrodynamic drag and gravitational force. With the increase of solids concentration in hindered settling region, the indirect interaction (hydrodynamic interaction) between particles leads to a deviation of the Stokes settling behavior (de Kretser et al., 2003). In the hindered settling factor approach, a volumetric friction-dependent hindered settling factor, $r(\varepsilon)$, is introduced to account for this deviation, and the hydrodynamic drag as follows:

$$F_d = \frac{\lambda_{st}\varepsilon r(\varepsilon)}{V_p(1-\varepsilon)}(v_s - v_l) \tag{21}$$

where η_s is the liquid viscosity, V_p is the particle volume. In the infinite dilution condition, $r(\varepsilon)$ approaches to zero to reflect the fact that the single particle sedimentation is unaffected by the neighboring particles. The maximum close packed concentration limits ε to less than 1, preventing $r(\varepsilon)$ from becoming infinite (de Kretser et al., 2003). Batchelor (1972) defined $r(\varepsilon)$ as a linear function of ε, while Buscall et al. (1982) showed that $r(\varepsilon)$ increases exponentially as the volumetric friction increases, and established the empirical relation based on experimental data curve fitting:

$$r(\varepsilon) = (1-\varepsilon)^{-4.5} \tag{22}$$

Given the fact that the most real systems are poly-disperse, and $r(\varepsilon)$ is invariably linked to the quantity λ_{st}/V_p, it is more convenient to measure $\lambda_{st}\, r(\varepsilon)/V_p$ as a whole, which is defined as the hindered settling function $R(\varepsilon)$ (de Kretser et al., 2001; Usher et al., 2001; de Kretser et al., 2003). The general formula of $R(\varepsilon)$ is shown as follows:

$$R(\varepsilon) = w(1-\varepsilon)^m \tag{23}$$

$$R(\varepsilon) = r_a\left(\varepsilon - r_g\right)^{r_n} + r_b \tag{24}$$

where w, m, r_a, r_b, r_n and r_b are empirical fitting parameters. Although $R(\varepsilon)$ is termed as the hindered settling function, it spans the entire concentration region, including the compression settling zone, to quantify the hydrodynamic drag associated with various settling behaviors. The experimental methods of characterizing $R(\varepsilon)$ specifically depend on the solids concentration: in the low to intermediate concentration range, a batch sedimentation test is the only available approach, while centrifugation and filtration techniques can be used over gel point to account for the compression effect (de Kretser et al., 2003).

If the internal flow approach is applied, the flow is regarded as a flow through a porous medium with limited permeability, and the upward water experiences more and more resistance with an increase of the solids concentration. The friction force experienced by a particle equals to that experienced by water, which can be determined by the Darcy's law:

$$F_d = K(\varepsilon)(v_s - v_l) \tag{25}$$

where $K(\varepsilon)$ is reciprocal of the hydraulic conductivity as a numerical equivalent of the hydrodynamic drag coefficient. It is a function of volumetric friction, and independent of the flow velocity (Zheng and Bagley, 1998). Zheng and Bagley (1998, 1999) defined an empirical function for $K(\varepsilon)$ based on the Vesilind equation as follows:

$$K(\varepsilon) = \frac{g\left(\rho_s - \rho_f\right)\varepsilon \exp(n_1\varepsilon)}{\rho_s k_1} \tag{26}$$

where n_1 and k_1 are Vesilind equation parameters, which can be determined by experiment data curve fitting approach. Another approach is to associate $K(\varepsilon)$ with certain physically meaningful variables for more theoretical formula derivation (Karl and Wells, 1999; Kinnear, 2002):

$$K(\varepsilon) = \frac{\mu\varepsilon}{k} \tag{27}$$

where μ and k are the liquid viscosity and intrinsic permeability, respectively. The intrinsic permeability, k, can be determined by either an empirical approach (Eq. (28)) (Dixon et al., 1976; Karl and Wells, 1999) or a theoretical formula (Eq. (29)) known as the Carman-Kozenny equation (Lee et al., 1996; Kinnear, 2002):

$$k(\varepsilon) = \alpha \exp(\beta\varepsilon) \tag{28}$$

$$k(\varepsilon) = \frac{\varepsilon^3}{5S_0^2(1-\varepsilon)^2} \tag{29}$$

where α and β are model parameters, S_0 is the specific surface area of the primary particle. Landman et al. (1988) demonstrated that the hindered settling factor approach and the Darcy's law approach only differ in the representation of the drag coefficient, but have a similar, even identical rheological basis.

The Kynch batch flux density (f_{bk}) refers to the flux density (εv_s) used in the mass continuity calculation based on Kynch's theory. The relationship between the Kynch batch flux density and the resistance coefficient ($\alpha(\varepsilon)$) is defined by Bürger et al. (2000a) as eq. (30):

$$f_{bk} = \frac{(\rho_s - \rho_l)g\varepsilon^2(1-\varepsilon)^2}{\alpha(\varepsilon)} \tag{30}$$

de Kretser et al. (2003) showed that the Kynch batch flux density and the hindered settling factor approaches are identical, differing only in nomenclature; f_{bk} can be related to the hindered settling function, $R(\varepsilon)$, by follows:

$$f_{bk} = \frac{(\rho_s - \rho_l)g\varepsilon(1-\varepsilon)^2}{R(\varepsilon)} \tag{31}$$

Therefore, similar experiment techniques including transient batch sedimentation test, centrifugal and filtration techniques can also be used for f_{bk} and $R(\varepsilon)$ determination. In conclusion, because of the similar rheological basis, the hindered settling factor approach, the Darcy's law approach and the Kynch batch flux density approach have are equally useful in determining the hydrodynamic drag coefficient, and the choice of approach strongly depends on experiment techniques and the available data sets.

3.2.3. *Compressive yield stress calculation*

When the suspension concentration exceeds the gel point where the self-supported network is formed to resist gravity and compression, the compressive yield stress arises from the unbouyed weight of the overlying particles, and is transmitted throughout the sediment to prevent the irreversible net framework collapse. Since the compressive yield stress only occurs over the gel point, proper methods are required to determine the gel point value before the compressive yield stress calculation.

As intrinsic properties, both the gel point and compressive yield stress depend implicitly upon the particle size, shape, the strength of aggregation, and the number, strength, arrangement of inter-particle bonds (Buscall, 1990; de Kretser et al., 2003). However, direct determination of the gel point still remains a problem because of its difficulty of measurement. For example, when the solids concentration at the top of the sludge blanket is at the gel point, the compressive yield forces present would raise the average bed solids above the gel point (Tien, 2002; de Kretser et al., 2003). Instead of considering the gel point as intrinsic property, Channell and Zukoski (1997) used the following constitutive function to define the gel point as a model parameter by the compressive yield stress curve fitting:

$$p_y = k\left(\left(\frac{\varepsilon}{\varepsilon_g}\right)^n - 1\right) \tag{32}$$

where k and n are parameters. This fitting approach should be applied with caution due to broad fit over a range of the gel point values (de Kretser et al., 2003). Since the gel point value could be a time-dependent value (Diplas and Papanicolaou, 1997; Kinnear, 2002; De Clercq, 2006; De Clercq et al., 2008), De Clercq et al. (2008) determined the gel point as the concentration where the concentration gradient becomes less than 200 g/l/m, a site specific value, within the sludge blanket rather than a certain gel point value. Other more theoretical methods based on the sediment equilibrium force balance are also available (Tiller and Khatib, 1984; Green, 1997), the estimated gel point, however, is still lower and more detailed study utilizing both shear and compressive techniques is required (de Kretser et al., 2003).

In most previous studies, the compressive yield stress is always expressed empirically as a function of solids concentration or solids volumetric concentration by using polynomial, power or exponential laws (Buscall and White, 1987; Auzerais et al., 1988, 1990; Buscall, 1990; Font, 1991; Bergstrom, 1992; Holdich and Butt, 1997; Karl and Wells, 1999; Bürger, 2000; Gustavsson and Oppelstrup, 2000; Kinnear, 2002). However, Zheng and Bagley (1998, 1999) suggested that the compressive yield stress is a function of both the solids concentration and the concentration change rate as Eq. (33) shows, which is in accordance with Dixon's hypothesis (Dixon, 1978).

$$p_y = k\frac{d\varepsilon}{dt}\frac{1}{\varepsilon} \tag{33}$$

where k is the model parameter. Hence, their compressive yield stress model greatly differs from the traditional concentration dependent models in the constant concentration region, such as the zone settling region. Because of the absence of a concentration gradient, Zheng and Bagley's model predicts zero compressive yield stress in constant concentration zones without making any additional assumption, as other models require. De Clercq et al. (2008) stated that the most frequently used power or exponential model cannot accurately describe the calculated compressive yield stress, especially for batch settling tests at high initial concentration. This deviation is attributed to the increasing gradient that exists at higher concentration, which do not conform to experiment observations. A logarithmic function with two parameters, α and β, is presented to overcome this shortcoming:

$$p_y = \alpha \ln\left(\frac{\varepsilon - \varepsilon_g + \beta}{\beta}\right) \tag{34}$$

Table 3 summarizes the mostly used compressive yield stress functions. Polynomial, exponential and power models are almost equivalent in compressive yield stress calculation, while the logarithmic model is developed to capture the logarithmic behavior of the stress that cannot be modeled by the other three.

4. Numerical technique discussion

For typical batch sedimentation modeling without considering the dispersion and compression effects, the model governing equation can be expressed as Eq. (1) as a combination of Kynch's assumption and the mass conservation law, that can be written as follows:

$$\frac{\partial \phi}{\partial t} + \frac{\partial (f_{bk}(\phi))}{\partial z} = 0 \tag{35}$$

The numerical challenge of solving this equation is the non-linear hyperbolic property. The dispersion and compression effects can be added, without increasing the complexity of solution, but have limited value unless the hyperbolic problem is first solved (Bürger et al., 2011). Therefore, Eq. (35) is generally used as the primary objective function in most numerical analysis studies (Kynch, 1952; Petty, 1975; Bustos, 1988; Bustos et al., 1990a, 1990b; Bustos and Concha, 1992; Diehl, 1996, 2000; Bürger et al., 2003,,2010; 2012). As a first-order nonlinear hyperbolic PDE, the solution to Eq. (35) is constant along the characteristic lines which are given by:

$$\frac{dz}{dt} = f'_{bk}(\phi) \tag{36}$$

Obviously, the characteristics are straight lines, which means a constant concentration ϕ_0 propagates with the speed $f'_{bk}(\phi_0)$ in a z-t coordinate plane. Two characteristics with different concentrations may intersect during the propagation and then a shock (solution discontinuity) occurs (Diehl, 2000). Kynch (1952) developed the first characteristics (iso-concentration line) analysis approach for batch sedimentation, and succeeded in capturing the shock (the interface of sediment and supernatant). Because of its great success in the sludge blanket level prediction, this characteristics analysis approach was further developed to build the framework of the well-known flux theory for SST design and operation investigations (Keinath et al., 1977; Keinath, 1985; Chancelier et al., 1997; Diehl, 2008). Petty (1975) extended Kynch's procedure to the continuous sedimentation, and provided an explicit shock analysis for the transient state, while Bustos et al. (1990a) constructed the global weak solutions based on the method of characteristics for various initial data and operating conditions. Diehl (2000) applied characteristic

Table 3 – Overview and comments of different compressive yield stress functions.

Compressive yield stress (effective stress)			
Model type	Model formula	Source	Comments
Polynomial model	$\phi = a + b\sigma_e + c\sigma_e^2 + d\sigma_e^3$	Font (1991)	≻empirical model;
Exponential model	$\sigma_e = a\,\exp^{(b\phi)}$	Karl and Wells (1999)	≻these models only differ in model formula, but almost identical in compressive yield stress approximation;
Power model	$\sigma_e = a((\phi/\phi_g) - 1)^b; \sigma_e = a((\phi/\phi_g)^b - 1)$	Landman et al. (1988)	≻some introduce the gel concentration or the maximum package concentration as model parameters;
	$\sigma_e = a\phi^b/(\phi_{\max} - \phi)$	Bergstrom (1992)	≻provide an increasing stress gradient for higher concentration range;
	$\sigma_e = (\phi/a)^b$	Holdich and Butt (1997)	
Logarithmic model	$\sigma_e = \alpha\,\ln((\phi - \phi_g + \beta)/\beta)$	De Clercq et al. (2008)	≻empirical model; ≻developed to capture the logarithmic behavior of σ_e which cannot modeled by the exponential or power models;

analysis to SST analysis with a further consideration of the impact of the converging cross-sectional area and various boundary conditions at top, bottom and inlet. As a conclusion, the method of characteristics or the characteristics analysis is currently the only available approach to obtain exact solutions of the nonlinear hyperbolic governing PDEs, however, it requires considerably more effort of its implementation in engineering practice, and further investigations are needed.

Because of the existence of solution discontinuities, Eq. (35) does not have closed-form solutions, and reliable numerical techniques are encouraged to produce approximate solutions that converges to the exact one as the grid mesh is refined (Bürger et al., 2011). To obtain both numerically and physically acceptable solutions, Eq. (35) cannot be straightforwardly discretized, and numerical schemes specially designed to solve the scalar conservation law equation are needed to satisfy three fundamental principles: the Courant-Friedrichs-Lewy condition (CFL condition) to ensure stability, the "consistent" numerical flux, a function of the concentration in neighboring layers, and the entropy condition to reject unphysical discontinuities. Great effort has been made to obtain a suitable numerical technique, and the earliest, but the most used one in environmental engineering field is the Stenstrom numerical flux, as shown in Eq. (12), which originated as a method for predicting solids overloading. Nevertheless, it may invalidate the entropy condition, and produces unphysical solutions which is demonstrated by Bürger et al. (2011) and Li and Stenstrom (2014b). Bürger et al. (2012) further showed that the Stenstrom flux is only sufficient for standard batch sedimentation and normal operation SST modeling, where the concentration is increasing as a function of the depth. The well-known Godunov numerical flux (F^G) was first introduced for SST simulation by Jeppsson and Diehl (1996), and also used by Plósz et al. (2007). The Godunov numerical flux in clarification zone can be shown as Eq. (37):

$$F^G_{i+\frac{1}{2}} = \begin{cases} \min\limits_{\phi_i \le \phi \le \phi_{i+1}} \left(v_s\phi - \dfrac{Q_e}{A}\phi \right) & \text{if } \phi_i \le \phi_{i+1} \\ \max\limits_{\phi_{i+1} \le \phi \le \phi_i} \left(v_s\phi - \dfrac{Q_e}{A}\phi \right) & \text{if } \phi_i > \phi_{i+1} \end{cases} \tag{37}$$

It is noticeable that the F^G differs from F^S in the flux calculation by including the bulk transport, and the concentration inverse situation where the concentration is decreasing as a function of the depth. Based on the Godunov numerical flux, Bürger et al. (2010) derived Method G, which is first-order correct. Another alternative method called Method EO, based on the Engquist-Osher numerical flux (Engquist and Osher, 1981) was developed by Bürger et al. (2005) and further refined by De Clercq et al. (2008).

Though both Method G and Method EO are reliable for SST modeling, and yield similar or identical solutions in many cases, their selection as a PDE solver is subjected to several competing principles: the complexity of implementation, the solution accuracy, and the computation cost which is indicated by the CPU time. The comparison study (Bürger et al., 2012) showed that the Method EO is too complicated for a straightforward application as the PDE solver in practical engineering cases, and for a given discretization level, the Method G is capable of producing acceptable and faster solutions than Method EO. However, Method EO reduces numerical error more efficiently than the Method G, which may favor Method EO for calculating of high accuracy numerical solutions.

The Godunov numerical flux and Engquist-Osher numerical flux are both monotonic, are only first-order accurate in shock capturing, Li and Stenstrom (2014a) improved the SST PDE solver by introducing a total variation diminishing (TVD) technique: the YEE-Roe-Davis flux limited scheme (Method YRD) (Yee et al., 1990). By imposing the solution difference calculation and flux limiter technique, the Yee-Roe-Davis technique is able to determine what to do in terms of the solution gradient but ensures the stability across the shock. Therefore, it is second-order correct in both smooth and discontinuous regions with small tradeoffs.

For the convection-dispersion model (Eq. (13)), including the dispersion term transforms the original nonlinear hyperbolic PDE to a parabolic PDE, which is significantly easier to solve numerically. David et al. (2009a, 2009b) proposed the Method of Lines (MOL) strategy for this problem, based on the use of finite difference methods and time integrators. Generally, MOL proceeds in two steps (David et al., 2009a):

1. approximating the spatial derivatives by using finite-difference or spectral methods;
2. the resulting system of semi-discrete (discrete in space but continuous in time) equations are integrated in time;

The efficiency and flexibility of MOL's implementation in practical analysis and control have been demonstrated by various numerical simulation tests of the convection-dispersion model.

When the compression effect term is imposed, the phenomenological analysis of the various settling materials yields a degenerate parabolic PDE model (Eq. (19)), which means the governing PDE is nonlinear hyperbolic if $\phi < \phi_g$, but nonlinear parabolic if $\phi > \phi_g$. Because of its mixed nonlinear hyperbolic-parabolic nature, the solution of the convection-compression model can also be discontinuous, hence making it difficultly to be discretized straightforwardly as in the convection-dispersion model case (Bürger et al., 2000b, 2006; Berres et al., 2003; Bürger et al., 2006). The developed Method G, Method EO and Method YRD can be used for the nonlinear convection term discretization, while for the nonlinear compression term discretization, if the primitive con not be expressed in closed form, it can be approximated by numerical integration (Bürger et al., 2013).

If the inertial effect is further considered, the complete model format is a mixed hyperbolic-parabolic equation system (Eqs. (15)–(18)). In Karl and Wells' approach (Karl and Wells, 1999), Eq. (16) was first solved to determine ϕ at the new time level $(n+1)$, and then, Eq. (18) was solved for v_s at the new time level $(n + 1)$ based on the solution of Eq. (16). An explicit upwind scheme was introduced to discrete Eq. (16) shown as follows:

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \frac{(\phi v_s)_{i+1/2}^n - (\phi v_s)_{i-1/2}^n}{\Delta z} \tag{38}$$

where n is the time index. Because this technique is unconditionally unstable for convection-dominate systems, Karl and Wells (1999) also added an artificial numerical diffusion term to smooth the shock during the calculation. The momentum equation (Eq. (18)) can be solved either implicitly or explicitly, as well as being discretized with either a central difference or upwind scheme. The numerical simulation tests showed that the fully explicit formula of the momentum equation needed a very small time step (Δt), which greatly increases computation cost, while the implicit method allows for larger time steps (Karl and Wells, 1999). The selection of the upwind or central difference methods does not seriously impact the final simulation solutions.

Table 4 summarizes most alternative techniques that can be used for accurate analytical or numerical solutions solving. Until now, none of these strategies can completely satisfy the requirement of high solution accuracy and low computation cost, and more studies are needed in the future to develop solution calculation technique, which is not only efficient in accurate solution calculation, but also easy for implementation in practical application.

5. Modeling challenges and perspectives

5.1. *Settleability determination*

Because of the hydrodynamic simplification (assumption 3), the most significant experimental issue in 1-D SST modeling is to investigate the sludge gravity settling behavior, often made more difficult by the inherent unpredictability of the biomass settling prosperities. In most academic studies and practical engineering applications, instead of comprehensively investigating the relationship between the settleability and various impact factors (particle size, sludge density, filaments or no filaments, etc), the widely known index: Sludge Volume Index (SVI, or other closely related indexes stirred SVI (SSVI), diluted SVI (DSVI)) is used to qualitatively characterize sludge settleability, because its measurement can be performed more easily and routinely than multiple batch settling tests. However, the attainable information in SVI measurement is very limited, and given the variability of sludge settling behavior, can rarely predict the necessary sludge settling characteristics (Ozinsky, 1994; Plósz et al., 2011).

Even though the SVI is often measured in practical SST studies and during plant operation, it cannot be directly used as a parameter in SST models. Efforts have been made to overcome this drawback, for example the correlation between SVI and parameters in hindered settling velocity functions such as the Vesilind velocity function, by using empirical relations to identify SST model parameters from the SVI information (Pitman, 1984; Daigger and Roper, 1985; Wahlberg and Keinath, 1988; Ozinsky, 1994; Giokas et al., 2003; Plósz et al., 2011). However, the universality of these empirical relations cannot be confirmed with available data sets: Giokas et al. (2003) found that SVI or SSVI can be used to accurately predict the parameter, k, in Eq. (4) which is inconsistent with the conclusion presented by Plósz et al. that k is practically independent to the SSVI (Plósz et al., 2011). This inconsistency can be attributed to the different experiment conditions and the lack of solid theoretical background of these empirical equations. Hence, for future work, the experiment conditions and methodology should be unified to provide comparable data sets, and the examination of various alternative empirical functions between SVI and settling velocity function parameters are needed based on the verification of each function with well-collected data sets. Alternative functions such as those listed in Table 1 equation to relate SVI to settling velocity, should be investigated, because the Vesilind equation may not be able to simultaneously predict setting behavior at low and high concentration using only two parameters.

The relation between SVI and settling in the compression zone is unclear, and there is no practical way of identifying compression characteristics from the SVI. Given that most compressive yield stress functions as shown in Table 3 are functions of the solids concentration, in a fashion similar to the settling velocity functions, correlating SVI with compressive yield stress function parameters might be attempted. However, several problems can be foreseen, for example 1) the standard SVI only requires the sludge sample to be settled for 30 min, which may not be long enough for sludge to be sufficiently condensed beyond the gel point to enter the compression zone; 2) the range of initial concentrations normally observed in the SVI test may be too low to produce observation in the compression zone, especially for the DSVI procedure; 3) the convenient equipment size associated the SVI test and lack of stirring maybe allow wall effects and bridging to produces erroneous results. Further experimental studies are encouraged to address these problems, thus

Table 4 – Overview and comments of different numerical techniques used in solving the model governing PDEs.

Numerical technique				
Model type	Formula type	Numerical method	Source	Comments
Convection model	Nonlinear hyperbolic PDE	Method of characteristics	Petty (1975)	≻Method of characteristics is the only available approach for analytical solution calculation, but it is difficult for implementation;
		Stenstrom flux constraint	Stenstrom (1976)	≻Stenstrom flux constraint is easy for implementation, but can be problematic in several situations, such as the negative concentration gradient condition;
		Godunov scheme (Method G)	Jeppsson and Diehl (1996)	≻Method G and EO converge to the physically relevant solutions, but only own first-order accuracy in both discontinuity and smooth regions;
		Engquist-Osher scheme (Method EO)	Bürger et al. (2005)	≻Method YRD converges to the physically relevant solutions, and owns second-order accuracy in both discontinuity and smooth regions;
		Yee-Roe-Davis scheme (Method YRD)	Li and Stenstrom (2014)	
Convection-Dispersion model	Linear parabolic PDE	Central-differencing scheme	Hamilton et al. (1992)	≻compared with the nonlinear hyperbolic PDE, adding the hydraulic dispersion term greatly reduces the complexity of the numerical solution calculation;
		Method of lines	David et al. (2009a)	≻Both central-differencing scheme and Method of lines are easy for implementation;
	Nonlinear parabolic PDE	Upwind scheme	Watts et al. (1996)	
Convection-compression model	Degenerate hyperbolic-parabolic PDE	Numerical techniques used for convection model solving is applicable for the convection term discretization; the conservative scheme is used for the compression term discretization;	Bürger et al. (2000) Berres et al. (2003) Bürger et al. (2006)	≻the model formula type is nonlinear hyperbolic if $\phi < \phi_g$, nonlinear parabolic if $\phi > \phi_g$; ≻the numerical techniques used for convection model are suitable for the convection term discretization, while the nonlinear compression term requires special conservative schemes;
		Operator splitting methods	Bürger et al. (2000)	≻for the compression term discretization, if the primitive cannot be expressed in closed form, it can be approximated by numerical integration;
Convection-dispersion-compression model	Mixed hyperbolic-parabolic PDE	Numerical techniques used for convection model solving is applicable for the convection term discretization; the conservative scheme is used for the compression term discretization; central differencing scheme is used for the hydrodynamic dispersion term discretization;	Bürger et al. (2011) Bürger et al. (2012) Bürger et al. (2013)	≻the model formula type is nonlinear hyperbolic if $\phi < \phi_g$, nonlinear parabolic if $\phi > \phi_g$; ≻solving this type of model requires the combination of the various numerical techniques used in the models discussed above;

making the compression parameters more available and understandable for practical engineering measurement.

5.2. Data availability and measurement techniques

High resolution data sets are required in SST modeling mainly for two reasons: 1) the empirical functions describing various settling behaviors require calibration, and 2) model validation and comparison.

Existing SST models strongly rely on empirical functions to describe various settling behaviors: the hindered settling velocity function to model the hindered settling process, and the compressive yield stress function to model the compression settling process. The methodology discussed in Section 2, including choosing appropriate cylinder size and slow mixing, initial sludge height are required to collect reliable hindered settling data. However, until now, there is no practically reliable method available to collect data outside of the zone settling range (Ekama and Marais, 2004), which means most experiment data sets fail to provide sufficient information or standardization to include other needed settling regions, such as the compression settling range. Although advanced methods such as medical computer tomography scanning (Auzerais et al., 1990) and radiotracing (De Clercq et al., 2005; Vanrolleghem et al., 2006; De Clercq et al., 2008), have been used to obtain high resolution concentration and compression pressure profiles during batch settling tests, their use as a routine test methodology is unlikely because of high complexity and cost. Researchers in future investigations should exercise great care when choosing empirical functions and collecting calibration data to insure that experimental errors do not unknowingly impact model performance.

In addition to problems arising from poorly calibrated empirical functions caused by the lack of well collected batch settling data, the difficulty of collecting full-scale, continuous SST data has created a situation where SST models are not sufficiently verified, and the evaluation of recently developed SST models cannot be clearly tested. As a compromise, in many publications, batch settling models, instead of continuous SST models are used to test model performance based on batch settling concentration profiles, since these two models mainly differ by including bulk transport, but have similar rheology foundations. However, if hydrodynamic dispersion function needs to be modeled, the batch settling concentration profile cannot be used in lieu of the full-scale concentration profile. The non-ideal hydrodynamic effects only be reliably observed in a full-scale SST. One solution presented by Plósz et al. (2007, 2011) is approximating the averaged 2-D CFD concentration profiles with the 1-D model predictions, so the hydrodynamic dispersion function can be calibrated over a wide range of flow conditions, and the model performance can be tested using the 2-D CFD model simulation results instead of real full-scale SST data sets. This method seems to be reliable and convenient, but further investigations are required to demonstrate its universality. Researchers can also use some available full-scale SST data sets such as Pflanz's data (Pflanz, 1969), Anderson's data (Anderson, 1981) including the hydrodynamic dispersion coefficient estimation, and Kinnear's data (Kinnear, 2002) including compressive yield stress function parameter estimation to evaluate the model performance.

5.3. Solution techniques

The nonlinear nature of the SST model formulas can prevent their straight forward discretization due to possible solution discontinuities. The equations most associated with SST modeling are two examples: the nonlinear hyperbolic PDE (convection dominant model) and the strongly degenerate parabolic PDE (convection-compression model). Therefore, reliable solution techniques are important for this modeling problem not just from a mathematical interest but also because they needed to produce accurate solutions. Table 4 shows various solution techniques, that have been developed, and their convergence to physically relevant solutions has been demonstrated. Practical engineers and researchers are able to select the most suitable method based on the model formula and needed solution accuracy, within the constraints of their computing facilities. More efficient solution techniques are always needed to keep up with advancing research needs as well as implementation into commercial simulators, which is still challenging. In addition to concerns for practical applications, renewed interest in different settling behavior may also require more advanced solution techniques. Most early SST models used nonlinear hyperbolic PDEs as the governing equation, since only hindered settling was considered. After having a better understanding of the compression settling process, a nonlinear diffusion term was added to simulate the compression effect, which changes the model formula from nonlinear hyperbolic to degenerate parabolic. Further study of sedimentation may make the governing equations more complex; for example the inconsistent conclusions of the importance of inertial effects may require its further investigation, which requires solving the whole PDE system (Eq. (15)–(18)) instead of the inertia-negligible model (Eq. (19)). Until now, there is no consensus for solution techniques to address this foreseeable question.

5.4. Settling behavior understanding

It is easy to recognize that the most significant but challenging task in SST modeling is the analysis of various settling behavior, and the development of the SST model should always be accompanied by the improved understanding of the settling process. In the most advanced convection-compression models, hindered settling is characterized by Kynch's assumption that the hindered settling velocity is only determined by local solids concentration, and compression zone modeling relies on the compression rheology assumption that the compressive yield stress within the compressed sediment is also a function of solids concentration. The verification of convection-compression SST models with batch and lab-scale continuous settling concentration profiles shows that these two approaches have achieved a degree of success in hindered and compression settling modeling (Bürger et al., 2000a). Nevertheless, some questions still remain to be answered:

1) Flocculent settling velocity determination: flocculation settling occurs in most full-scale SSTs, and greatly impacts the effluent solids concentration. However, because of the difficulty of physically observing interface height change in batch settling tests at low initial concentrations (~500 mg/L or less), tests at low concentrations are rarely performed. Continuous tests at these concentrations are also rarely performed, since few activated sludge processes operate at such low concentrations. To estimate settling velocities for the overall concentration domain, hindered velocity equations are extrapolated into the flocculation regime, and may produce unrealistic results (Kinnear, 2002). Hence, reliable flocculation velocity models are needed to provide more accurate predictions, such as the effluent solids concentration.
2) Changeable compressibility: Predicting accurate behavior in the transition zone between hindered and compression is challenging, as noted by Kinnear (2002), who observed that his improved convection-compression model, even when accurately calibrated with experimental data, provided accurate predictions only for the hindered and compression interfaces, and failed to accurately predict transitional behavior. Kinnear (2002). Attributed this problem to the changing sludge compressibility as a function of the shear history or flocculation state that makes the gel concentration vary. This same conclusion was later supported by De Clercq et al. (2008). Given the importance of this assumption and its impact on compression modeling, additional experimental investigation is a high priority.
3) Transient settling behavior understanding: Inaccuracies in predicting observed transient settling interface height have been reported by two researchers (Kinnear, 2002; Stricker et al., 2007). This error can be attributed to the changeable compressibility as discussed above. Another plausible explanation is the lack of required degrees of freedom in the model formula to accurately describe transient settling behavior, as a result of insufficient understanding. The formation mechanisms of the transient settling zone remain unclear, and the intrinsic instability of the transient zone itself impedes analysis, both experimentally and theoretically. However, if we review the reason for Kynch's assumption, he said "a considerable amount can be learned by a single main assumption without knowing the details of the forces on the particles". The success of this approach in making assumptions in lieu of a complete theoretical understanding of hindered settling suggests that it may also be useful to introduce an assumption for the transient settling investigation. One potential new starting-point of the transient zone study can be Dixon's (1977a) assumption that the overall acting force in transient settling can be approximated as a function of solids concentration and the settling velocity change rate.

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