Computational Simulation of Flocculent Sedimentation Based on Experimental Results

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Abstract

Computerised interpolation algorithms as well as the empirical model for analysing the flocculent settling data were developed. A mechanistic semi-empirical model developed from fundamental physical principles of a falling particle in a viscous fluid was tested against actual flocculation column data. The accuracy of the mechanistic model was evaluated using the sum of the squared errors between the interpolated values (real values) and the model predictions. Its fitting capabilities were compared with Özer's model using nine flocculent data sets of which four were obtained from literature and the rest was actual data from the performed experiments. The developed model consistently simulated the flocculation behaviour of particles in settling columns better than Özer's model in eight of the nine data sets considered. It is recommended that the model's performance be further compared with other models like the Rule based and San's model. The errors due to the use of interpolated values when determining the performance of the empirical models need to be investigated. Furthermore, a three-way rather than two-way interpolation should now be achievable using the interpolation algorithm developed in this study thereby reducing the effects of interpolation bias. The above work opens the way to full automation of design of flocculation sedimentation basins and other gravitational particle separation systems which at present are designed manually and are susceptible to a wide range of human and random errors.

Keywords: sedimentation, flocculation, total suspended solids, iso-percentile profiles, empirical modelling, automated design.

INTRODUCTION

During the design of flocculent sedimentation tanks, data from settling column tests is interpreted by a graphical technique. Samples at different times and depths are analysed for suspended solids concentration and removal rate profiles are manually plotted as a function of time. From the graphs, one can predict or calculate the removal efficiency, overflow rate, and settling velocities. The results from the graphs are then used to determine the desired sedimentation tank parameters. The obvious shortcoming of this procedure is that no two individuals can end up with the exact same design and the process is in itself tedious. In addition to the problem of irreproducibility, the graphical method is sometimes misleading in the region of less variability typically at the beginning of the settling process (San, 1989).

Another approach that has been tried is by using mathematical models (simulations) which do not require the experimental data. An earlier example is by Takacs et al. (1991) who proposed a model for predicting the solids profiles along the settling column based on the mass balance around each layer of a one dimensional settler. In the model by Takacs and coworkers, an attempt is made to link removal to settling velocities to include the effect of thickening of the solution as particles settle. This is represented by the following equation:

$$v_{sj} = v_0 e^{-r_h Xj^*} - v_0 e^{-r_p Xj^*} \tag{1}$$

$$0 \le v_{sj} \le v_0^{'} \tag{2}$$

where v_{sj} =settling velocity of solid particles in a layer j (LT^{-1}), v_0 = maximum terminal velocity of particles (LT^{-1}), r_h = settling parameter characteristic of the hindered settling zone (L^3M^{-1}), r_p = settling parameter characteristic of the low solids concentration (L^3M^{-1}), $X_j^* = X_j – X_{\min}$, where X_j = suspended solids concentration in layer j (ML^{-3}), and $X_{\min}$ = minimum attainable suspended solids concentration (ML^{-3}).

The model by Takacs has been tested on the settling of thick solutions such as settling of mixed liquor suspended solids (*MLSS*) in secondary clarifiers. Application in dilute solutions such as potable water sedimentation basins is limited by the unreliability of the data collected from settling columns collected during the first few minutes which increases the error in the r_p parameter in Equation 1. Notably, the application of purely theoretical models is mostly limited by the variations in physical conditions in non-ideal sample solutions which are difficult to represent mathematically (Martínez-González et al, 2009).

In this study, a semi-empirical mechanistic model is derived for analysis of physical data from settling columns. The model aims to achieve a robust algorithm simulation of particle removal trajectories from column test data. According to Kynch (1952), the concentration of total suspended solids (TSS) remaining in solution at layer j (X_j) should be a function of time t (T) and depth D (L) (Kynch, 1952), i.e.:

$$X_j = f(t, D) \tag{3}$$

However, the model is valid only when the following boundary conditions and assumptions are satisfied (Je *et al.*, 2002):

(a) Settling is only occurring only in the direction of velocity.

$$\frac{\partial D}{dt} \geq 0 \tag{4}$$

(b) The solution is thickening with the increase in depth.

$$\frac{\partial X}{dD} \geq 0 \tag{5}$$

(c) Removal is achieved in all layers, i.e., no compression stage has been achieved in all layers.

$$\frac{\partial X}{dt} \geq 0 \tag{6}$$

(d) Variations of TSS concentration remaining should not increase with depth.

$$\frac{\partial^2 X}{dD^2} \geq 0 \tag{7}$$

Mathematical constraints of the regression parameters based on the physics of flocculent settling curves are represented by the conditions stated above (Equation 3 to 7). Some of the earlier proposed implementation of the flocculent particle sedimentation model, such as the Berthouex and Stevens' model, violated the above mathematical criterion at long-settling times. The best simulation results have so far been obtained using the two semi-mechanistic (rule-based) models, i.e., the Özer's model:

$$P = \alpha_1 D^{\alpha_2} t^{\alpha_3} \tag{8}$$

$$1 + P = A_1 D^{A_2} t^{A_3} \tag{9}$$

where P = percentage removal $(1\text{-}X_j/X_o)\times 100$, X_o = initial concentration in the column (ML^{-3}), D = depth travelled by particle during settling (L), and t = time of settling (T). The percentage removal is a function of depth D and time T through the relation in X_j (Equation 3). The San's model:

$$P = \frac{t^{\beta}}{\alpha D^{k} + t^{\beta}} \tag{10}$$

was derived as a variation of the Özer's model. In Özer's model, the parameters α_1, α_2, α_3, A_1, A_2, and A_3 = mechanistic fit parameters for the iso-percentile lines. The fitting parameters in San's model are α, β, and k. San's and Özer's have been shown to comply with the as assumptions stated in Equations 3 to 7 (Je *et al.*, 2002).

From the above, a modified rule-based model was developed to evaluate of settling column data as shown latter in this paper under the materials and methods. The final results and reliability of the model was heavily dependent on optimised parameters α_i, β and A_i also optimised based on the column test data.

MATERIALS AND METHODS

Standard Batch Settling Column

Figure 1 shows a simple batch column that was used in the collection of physical data. A 100 L mixing tank was used together with a stirrer to mix water with aluminium sulphate (coagulant) and dry clay soil. A 5 L beaker was used to transfer the dilute suspension from the mixing tank to the column. Sampling bottles were used to withdraw samples from the column at a given time.

Simulation of Dirty Water

90 L of water was poured into the mixing tank and approximately 400 g of dry clay soil was added to make the water dirty. The coagulant (aluminium sulphate) was then added and the stirrer was then switched on for 2 min at 180 rpm. On average, 20 min was allowed for large suspended solids to settle down in the mixing tank before transferring the solution to the experimental settling column. The colloidal suspension was then carefully transferred into the test column. Immediately after filling the column, two minutes were allowed before starting the 90 minutes of settling time. Samples from the 7 sampling ports were withdrawn at 0, 10, 20, 30, 45, 60, 75 and 90 min. Table 1 shows the experiments that were performed. Settling tests were conducted using five different ferric

chloride ($FeCl_3$) coagulant doses as shown in Table 1. Only representative date form the most effective dose (10 mg/L) is represented in this paper.

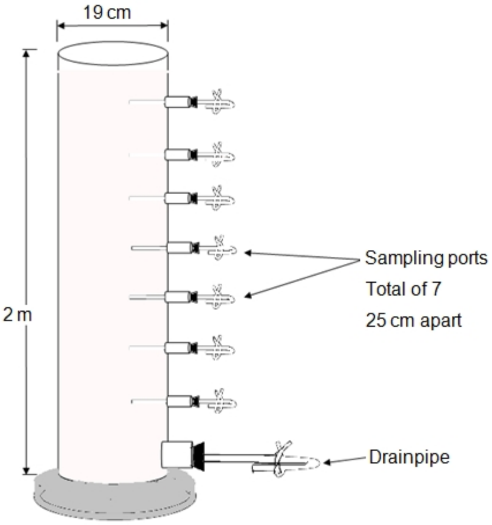

Figure 1. Settling column test

Table 1: Batch settling column experiments performed.

Experiment No.	Coagulant concentration (mg/L)	Average initial solids concentration (NTU)
1	10	195
2	50	208
3	70	170
4	68	112
5	70	141

Samples were analysed by a HACH Turbidity Meter (Model 2100N, Hach Company, Loveland, CO) and the recorded values in NTU's were converted to the mass concentration using the equation ln(TSS) = 1.5·ln(NTU)+0.15 based on the 10 point calibration line from a TSS versus NTU data ($R^2 = 0.97$) (Packman *et al.*, 1999). The total suspended solids (TSS) was measured in the range 10-300 mg/L as dry weight of suspended solids trapped on a 0.45 μm micro-pore membrane filter (APHA, 2005).

Data Analysis: Iso-Percentile Plots

Data analysis was carried out with the aid of the programming software platform, Octave (GNU Octave Version 3.4.2, Free Software Foundation, Boston, MA). An interpolation algorithm was generated and then computerised to plot the iso-percentage, profiles as a function of depth and retention time. A model for fitting these profiles was then developed and validated using the physical behaviour of flocculent particles. The Interpolate (T_j, T_{j+1}) or Interpolate (H_i, H_{i+1}) on the chart (Figure 2) refer to linear interpolation between two consecutive time points or heights to approximate the time or height at which a certain percentage removal value can be obtained.

Individual iso-percentile removal profiles were calculated from the geometrical relationship between the percentage removal and column height at any particular time as follows:

$$H_i = H_{\max} + r_1 P t^{r_2} \tag{11}$$

where r_1 and r_2 are semi-empirical optimisable parameters, H_i = height of sampling points, $H_{\max}$ = design height of proposed tank, and P = percentage removal $(1-X_j/X_o)\times100$.

The model was later modified to the final form (Equation 12) with an additional fitness parameter r_3 based on best fit analysis:

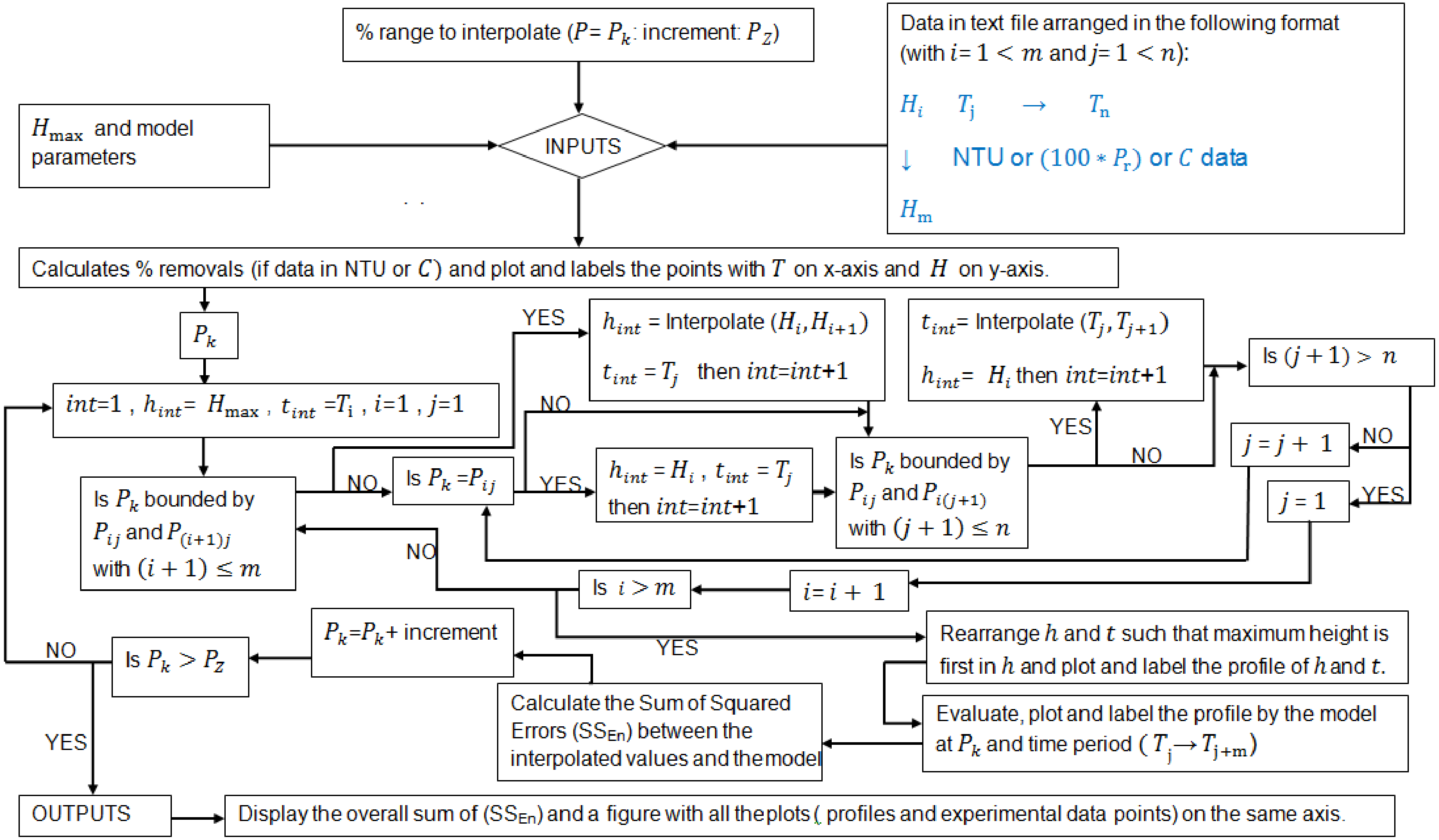

Figure 2: Flow chart representation of the algorithms used to generate the Octave program.

$$H_i = H_{\max} + r_1 P^2 t^{r_2} - r_3 P^2 t \tag{12}$$

Equation 12 can be rearranged and written as follows with the full range of parameters:

$$P = \left(\frac{-D}{r_1 t^{r_2} - r_3 t} \right)^{0.5} \tag{13}$$

$$D = H_{\max} - H_i \tag{14}$$

$$r_1 < 0 \tag{15}$$

$$r_2 > 0 \tag{16}$$

$$0 \le r_3 \sim \frac{0.1}{r_2} \tag{17}$$

The right hand side of Equation 17 was used as a first guess of the value of r_3.

RESULTS AND DISCUSSION

Evaluation of Settling Data

Data was collected from settling columns in experiments run for 90 minutes in columns ranging from 2.5 to 4 meters deep. An example of the results from an optimum dose of 10 mg/L $FeCl_2$ is shown in Table 2. The results collected were characteristic of most data from similar water samples. Examples are found in a range of technical texts including MetCalf and Eddy (2003), Reynolds and Richards (1996), Sawyer et al. (2003), and others. The conventional methods of analysing these data is by calculating percentage removals (usually by spreadsheet), plotting interpolation points, followed by plotting smoothed iso-percentile lines. The experimental data after calculating the percentage removals is shown as circles in the plots in Figures 3 and 4.

Table 2: Suspended solids concentration data from settling column test at X_o = 195±2 mg/L (coagulant dose = 10 mg/L $FeCl_2$)

Depth	**Concentration at Different Times**						
(m)	**10 min**	**20 min**	**30 min**	**45 min**	**60 min**	**75 min**	**90 min**
0.25	189	176	160	132	115	113	111
0.50	181	179	161	151	143	133	122
0.75	184	178	170	163	148	137	125
1.00	182	185	173	159	150	143	133
1.25	191	191	187	171	151	141	135
1.50	192	182	175	166	154	141	136
1.75	195	184	180	174	155	144	137
2.00	196	188	185	181	158	148	140
2.50	194	190	187	180	163	155	143

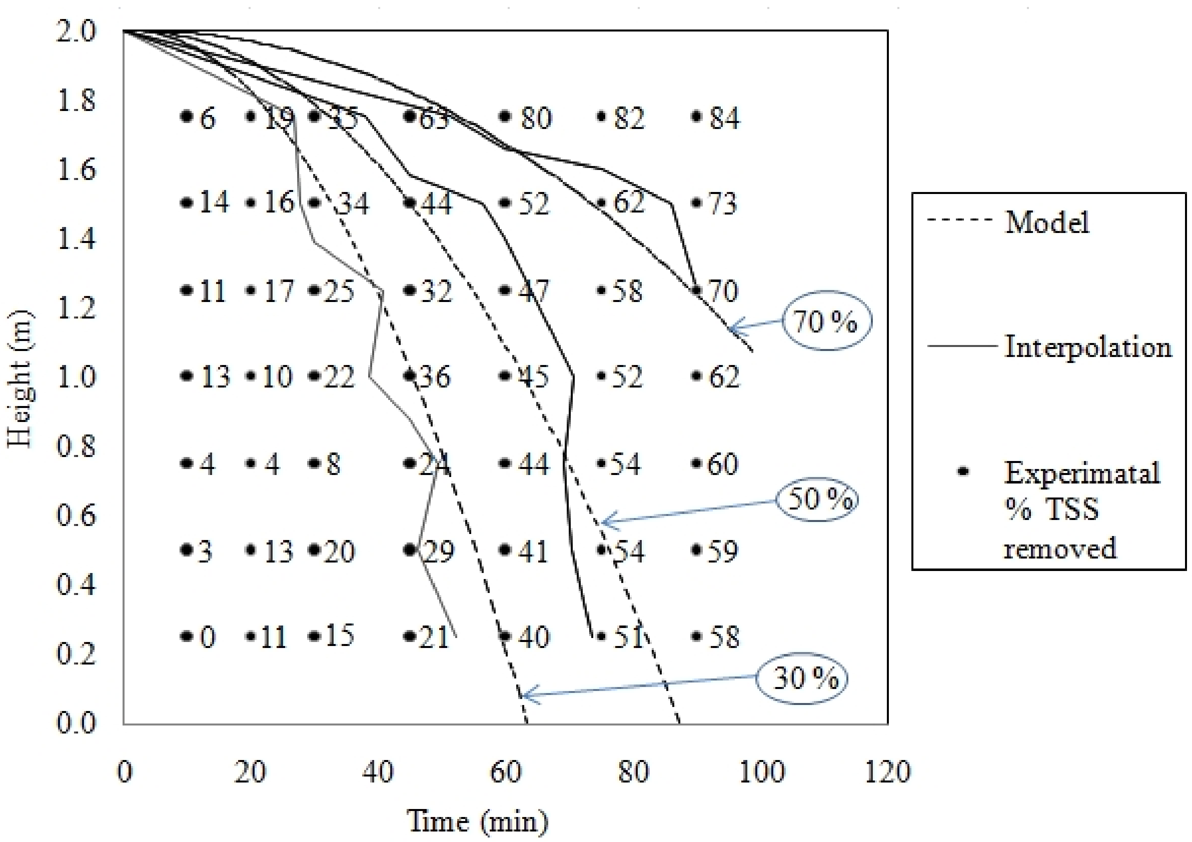

Figure 3: Interpolation results and iso-percentile removal profiles from the first experimental data.

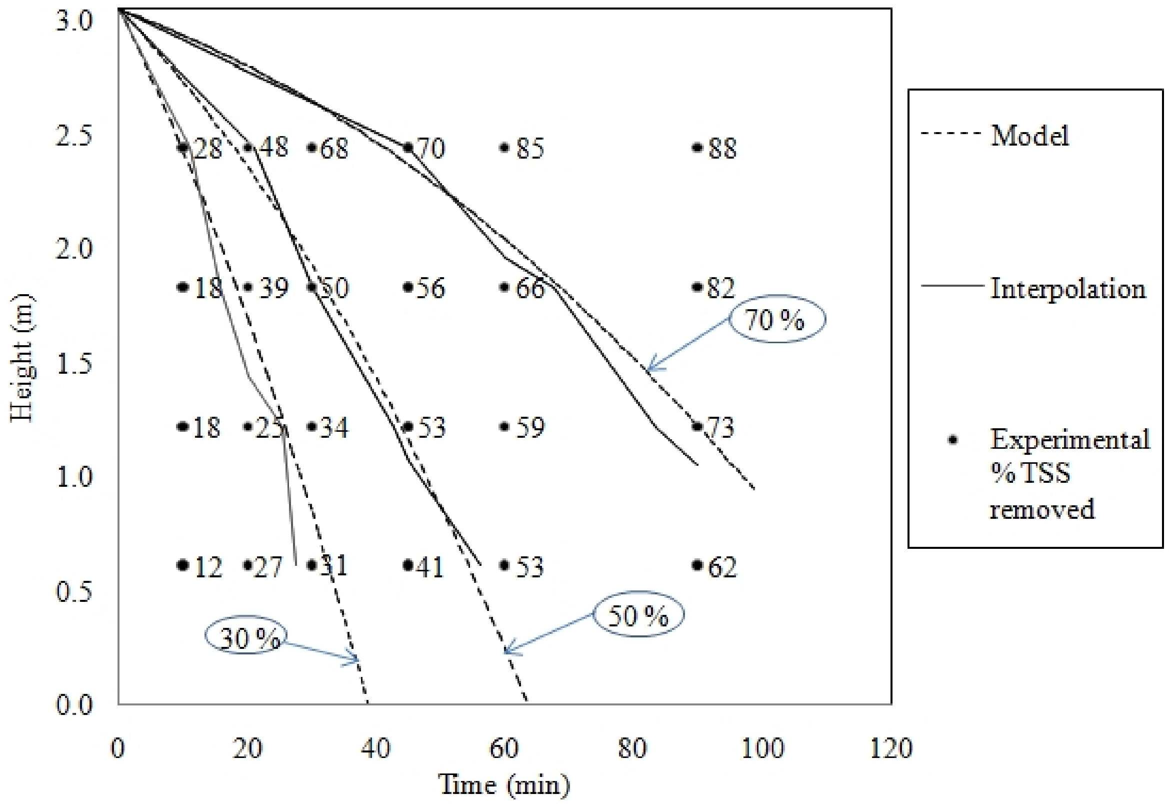

Figure 4: Interpolation results and iso-percentile removal profiles from the second experimental data.

Interpolation and Simulation

Before simulation of iso-percentile lines, the computational algorithm was used to generate the raw percentage removal data points using an interpolation routine presented in Figure 2. Normally, this exercise is done by hand in the real industry. The automated interpolation was conducted across the grid in the zero and ninety degree directions from a given data point. The accuracy of the interpolated data set is critical to the accuracy of the final percentiles since these provide the fixed scaffold points for the final analysis. For this reason, the improvement of the interpolation procedure is regarded in this study as the key to achieving the parameters of the highest possible accuracy for physical design of clarifiers.

The model presented in Equations 11 and 12 was then used to provide the smooth lines to approximate the trajectory of constant percentage removal. The model was tested against data collected in the laboratory and previous data presented in textbooks. Data from the textbooks in the stipulated range 300-800 mg/L was tested. Representative date from practical data collected in the laboratory is presented for example in Figures 3 and 4.

Typically, iso-percentile plots do not fit all areas of the data equally well. In practice, the accuracy of the interpolation is only seen after simulation of the whole data set and is evaluated holistically. This process can be improved by including two or more data points from the surrounding iso-percentile line in establish a point and use statistical means to improve accuracy.

In the given example data set, it is clear that the percentage removal profiles underestimate the observed removal profiles in the top three ports of the column and in the first 30 minutes in both data sets (Figure 3 and 4). The reason may be because in sufficient flocculation may have occurred in the first few minutes for the particles to behave in the manner consisted with a theoretical flocculent particle.

Error Analysis

In order to check the accuracy or performance of the model, the interpolated values were used as the real values and compared with the predicted values. An earlier study by Je and Kim (2002) observed better performance of mechanistic models over empirical models under certain data ranges. The lack of fit of empirical models was later attributed to limited range as they failed to approximate data around the outer boundaries of the calibrated areas. Another semi-empirical model, the Berthouex and Stevens' model, was the second best for fitting the data but it was later rejected since it violates assumption (b) and (c) of flocculent settling (Equations 5 and 6).

The fitting of the datasets was conducted firstly with Özer's model since it is consistent with the physical basis of flocculent sedimentation. The best fit of the literature based models was obtained from the San's model (Je and Kim, 2002). However, only the results from the modified model derived in this study are presented here. The model fitness is determined by the statistical data presented in Tables 3 and 4.

Visual inspection of the iso-percentile computations using the semi-empirical model derived in this study show that proposed model achieve a reasonably accurate representation of the percent removals. The general trends from the curve fitting with the Özer's and San's models were similar, thus, only the summary of the statistical comparison of the results are presented (Tables 3 and 4). Comparison of the sum of squares error (SS_E) between the fit from Equation 13 and Özer's model (Tables 3), shows that the proposed model performed better than the Özer's model for the data produced in the laboratory. For an unknown reason, the Özer's model produced a better fit from literature. The initial concentration of suspended solids in the literature data was almost an order of magnitude higher than the initial concentration in the measured data, i.e., X_o = approximately 200 mg/L in experimental data and approximately 800 mg/L in the tested literature data, respectively. This probably affected compaction factors resulting in different settling behaviour that was better captured by the mechanistic model.

Table 3: Sum of squared errors (SS_E) and parameters for the experimental data

	Proposed model				**Özer's model**			
Experiment No.	r_1 ($x10^{-3}$)	r_2	r_3 ($x10^{-3}$)	SS_E	a_1	a_2	a_3	SS_E
1	-0,94	2,141	0,00328	**3,62**	4,1	0,45	-0,53	**9,58**
2	-0,7	2,09	0,000041	**1,71**	4,35	0,46	-0,512	**3,23**
3	-0,7501	2,2	0,02911	**3,58**	4,5	0,69	-0,56	**8,59**
4	-0,751	2,048	0,01681	**1,71**	4	0,5	-0,48	**4,65**
5	-1	2,4	15,7	**3,52**	2,8	0,65	-0,51	**13,54**

Table 4: Sum of squared errors (SS_E) and parameters for the literature data

	Proposed model				**Özer's model**			
Data Source	r_1 ($x10^{-3}$)	r_2	r_3 ($x10^{-3}$)	SS_E	a_1	a_2	a_3	SS_E
Je *et al* (2007)	-1,3	1,64	71	**1,31**	2,439	0,55	-0,441	**1,34**
Reynolds & Richards (1996)	-0,76	2,101	118	**1,49**	1,91	0,55	-0,44	**3,72**
Berthouex & Stevens (1982)	-1,12	2,307	540,8	**1,55**	1,938	0,250	-0,633	**0,85**
Eckenfelder (1989)	-0,002	1,0009	79	**6,16**	2,365	0,46	-0,428	**6,70**

Model Validity

For the experimental data collected from the laboratory in this study, the order of performance was found to be proposed model > Özer's model > Berthouex and Stevens' model. At higher initial concentrations, the Özer's model outperforms the proposed semi-empirical model such that Özer's model > proposed model > Berthouex and Stevens' model. The results suggest that a rule-based (mechanistic model) is suitable for highly variable conditions whereas the more empirical approach is sufficient for more dilute solutions. For the model to work, it must comply with the conditions stipulated Equations 3 to 7 and constraints stipulated in Equations 14-17.

CONCLUSION

Human errors due interpolation by hand can be minimised by using reliable interpolation/optimisation algorithms to evaluate settling column data. In this study, an improved model that performed better than Özer's model in interpreting settling column data was developed. Automation of data analysis will enable engineers and scientists to perform three-way or four-way data interpolation of settling column data that will further improve design accuracy.

NOMENCLATURES

α	fitting parameter in San's model (dimensionless)
α_i	the model fitting parameters in Özer's model (dimensionless) (i = 1, 2, and 3)
β	fitting parameter in San's model (dimensionless)
A_i	the model fitting parameters in Özer's model (dimensionless) (i = 1, 2, and 3)
D	depth travelled by particle during settling (L)
H	ordinate representing depth
k	fitting parameter in San's model (dimensionless)
P	percentage removal $(1-X_j/X_o)\times 100$
r_i	semi-empirical optimisable parameters for proposed model (i = 1, 2, and 3)
r_h	settling parameter characteristic of the hindered settling zone (L^3M^{-1})
r_p	settling parameter characteristic of the low solids concentration (L^3M^{-1})
t	time of settling (T)
T	ordinate representing time
v	settling velocity (LT^{-1})
X_j	suspended solids concentration in layer j (ML^{-3})
X_{min}	minimum attainable suspended solids concentration (ML^{-3})
X_o	initial concentration in the column (ML^{-3})

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REFERENCES

APHA, 2005. Standard Methods for the Examination of Water and Wastewater. 21st Edition (Centennial Edition). By Eaton, A.D., Clesceri, L.S., Rice, E.W., Greenberg, A.E., Franson, M.A.H., (Eds.). American Public Health Association, American Water Works Association, Water Environment Federation, USA.

Berthouex, P.M. and Stevens, D.K. (1982). Computer Analysis of Settling Data. *ASCE Journal of Environmental Engineering*, 108(5), 1065-1069.

Christoulas, D.G., Yannakopoulos, P.H. and Andreadakis, A.D. (1998). An empirical model for primary sedimentation of sewage. *Environment International*, 24 (8), 925-934

Eckenfelder, W.W. (1989). *Industrial water pollution control,* 2nd ed., McGraw-Hill, New York, U.S.A.

Je, C. and Chang, S. (2004). Simple approach to estimate flocculent settling velocity in a dilute suspension. *Environmental Geology*, 45, 1002-1009.

Je, C., Hayes, D.F. and Kim, K. (2007). Simulation of resuspended sediments resulting from dredging operations by a numerical flocculent transport model. *Chemosphere.* 70, 187-195.

Je, C. and Kim, K. (2002). Evaluation of mathematical models for analyzing flocculent settling data *Environmental Progress,* 21(4), 255-264.

Kynch, G.J (1952), A theory of sedimentation, *Transcendental Faraday Society*, 48, 166-176.

Martínez-González, G., Loría-Molina, H., Taboada-López, D., Ramírez-Rodríguez, F., Navarrete-Bolaños, J.L. and Jiménez-Islas, H. (2009). Approximate method for designing a primary settling tank for wastewater treatment. *Industrial Engineering and Chemistry Research,* 48(16), 7842-7846.

MetCalf and Eddy (2003). Wastewater Engineering. Fourth Edition. Tchobanoglous, G., Burton, F., and Stensel, H.D. (Eds.), Metcalf & Eddy, Inc., McGraw-Hill, New York.

Özer, A. (1994). Simple equations to express settling column data. *ASCE Journal of Environmental Engineering*, 120, 677-682.

Packman, J.J., Comings, K.J. and Booth, D.B. (1999). Using turbidity to determine total suspended solids in urbanizing streams in the Puget lowlands: In Confronting Uncertainty: Managing Change in Water Resources and the Environment, Canadian Water Resources Association annual meeting, Vancouver, BC, 27–29 October 1999, p. 158–165.

Peavy, H.S., Rowe, D.R. and Tchobanoglous, G. (1985). *Environmental Engineering*, McGraw-Hill, New York, U.S.A.

Reynolds, T.D. and Richards, P.A. (1996). *Unit Operations and Process in Environmental Engineering*, 2nd ed., International Thomson Publishing, New York, U.S.A.

San, H.A. (1989). Analytical approach for evaluation of settling column data. *ASCE Journal of Environmental Engineering*, 115 (2), 455-461.

Sawyer, C.N., McCarthy, P.L., and Parkin, G.F. (2003), Chemistry for Environmental Engineering, Fifth Edition, McGraw-Hill, New York.

Takacs, I., Patry, G.G and Nolasco, D. (1991), A dynamic model of the clarification-thickening process. *Water Research*, 25(10), 1263-1271.

Wu, J. and He, C. (2010). Experimental and modelling investigation of sewage solids sedimentation based on particle size distribution and fractal dimension. *International Journal of Environmental Science and Technology*, 7 (1), 37-46.