# Modeling of a reactive primary clarifier

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**Abstract** Even though many models have been proposed for primary clarification, none is directly compatible with the ASM1. The objective of this paper is to present the development of a reactive primary clarifier model to be used in a wastewater treatment plant simulator (WEST). A model simulating COD behavior has been developed based on the Takacs model, and was tested with full-scale data. Particulate effluent COD was well described but problems occurred predicting the underflow suspended solids concentration. The model had to be upgraded with a residence time and a flocculation term to simulate the behavior of soluble COD. An ammonification term was added to the model, resulting in an improved model fit on effluent ammonium.

**Keywords** Ammonification; ammonium; ASM1; chemical oxygen demand; primary clarifier model

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## Introduction

The main objective of a primary clarifier in a wastewater treatment plant (WWTP) is to remove particulate matter from the influent raw sewage. The efficiency of its operation influences directly the subsequent biological and sludge treatment units. The understanding of the dynamics of primary clarifiers is, indeed, important to the overall effectiveness of the treatment plant (e.g. Lindeborg *et al.*, 1996). Moreover, in the wider context of river basin management, the performance of the primary clarifiers can dictate whether or not wastewater has to be discharged into the receiving river (Lessard and Beck, 1988).

Many models have been proposed to describe the behavior of primary clarification (Lessard and Beck, 1991). Primary clarification is often considered as being not very "sensitive", resulting in the use of simplified models to represent its dynamic behavior (Otterpohl and Freund, 1992). Most of the primary clarifier models do not consider any biological reactions to occur in the reactor, simulating only the suspended solids (SS) behavior. Moreover, these models seldomly use the same variables as those defined in Activated Sludge Model No.1 (ASM1; Henze *et al.*, 1987), and as a result, they are not compatible with a generally applied model such as ASM1. However, in certain cases some biological phenomena take place in the settlers (e.g. Lessard and Beck, 1988). Examples are primary clarifiers with high hydraulic retention times (retention times are sometimes more than six hours), clarifiers where anaerobic digester supernatant is recycled in the primary settler influent, or situations where excess biological sludge is combined with the plant influent to settle in the primary clarifier. Incorporation of biological reactions such as ammonification or hydrolysis in a primary clarifier model, could obviously lead to a better representation of the clarification process and of the global WWTP behavior.

The objective of this paper is to present the development of a reactive primary clarifier model to be used in a wastewater treatment plant simulator (WEST; Hemmis NV, Kortrijk, Belgium). Emphasis will be put here on the improved representation of the behavior of particulate and soluble COD in the primary clarifier.

## Methods

### The model

The developed model is based on the Takacs clarifier model (Takacs *et al.*, 1991) which is frequently used to describe the dynamic behavior of settlers. In the original WEST model, our starting point for this study, the Takacs clarifier model was used. However, the resulting soluble component concentration in the effluent of the clarifier was identical to the concentration in the influent as no time delay was included.

Basically the settler is divided into a number of layers (usually ten) and a mass balance is made over each layer to evaluate the SS profile in the settler. The particularity of the model is the use of a settling velocity model describing both clarification and thickening (Eq. 1):

$$v_{sj} = v_0 e^{-r_h X_j^*} - v_0 e^{-r_p X_j^*} \qquad 0 \le y_{si} \le v_{00} \tag{1}$$

where: $v_{sj}$ = settling velocity of the solids in the layer $j$ (m/d); $v_0$ = maximum Vesilind settling velocity (m/d); $v_{00}$ = maximum practical settling velocity (m/d); $r_h$ = hindered settling parameter ($m^3$/g); $r_p$ = flocculent settling parameter ($m^3$/g); $X_j^* = X_j - X_{\min}$ ($X_j$ = SS concentration in layer $j$ (g/$m^3$); $X_{\min} = f_{ns} X_{in;}$ $f_{ns}$ = non-settleable fraction of $X_{in}$ and $X_{in}$ = influent SS concentration (g/$m^3$)).

### The data

The data used to develop and validate the model are those obtained from a 10-day measurement campaign on the Norwich treatment plant (Lessard and Beck, 1988). Besides providing a complete database for a primary clarifier model evaluation, the data clearly show the presence of phenomena like degradation or flocculation of filtered COD, and ammonification (Lessard and Beck, 1988).

### Influent fractions

The average influent SS concentration of the available data set was 351 g SS/$m^3$. Knowing that only total and filtered COD ($COD_T$ and $COD_F$) were measured, some assumptions had to be made for the influent to convert measured COD values into an influent fractionation according to ASM1 variables: $S_S$ , $S_I$ , $X_S$ , $X_I$ . Filtered COD contains all the particles <1.2 μm while soluble COD contains the particles < 0.45 μm. According to Levine *et al.* (1991), the fraction of organic matter contained in the following particle size range, 0.001–1 μm, is around 15%. Considering this, and also keeping in mind our modeling objective, filtered COD was considered as soluble COD for the evaluation of the developed models. The COD influent fractions applied here were:

$S_I = 0.4\ COD_S$; $S_S = 0.6\ COD_S$; $X_I = 0.2\ COD_X$; $X_S = 0.8 COD_X$

where:

$COD_S = COD_F = S_S + S_I$ = soluble COD;

$COD_X = COD_T - COD_F = X_S + X_I$ = particulate COD.

No $X_{BH}$, $X_{BA}$ and $X_P$ were assumed present in the influent.

### Settling parameters

A first set of settling parameters were taken from Coderre (1999) and used as reference values (Table 1).

### Evaluation of model fit

Parameter fitting was done by minimizing the sum of squared errors between model predictions and data. The quality of the fit between simulated values and available data was also

**Table 1** Takacs settling parameters taken from Coderre (1999)

| Settling parameter | Value | Settling parameter | Value |
|---|---|---|---|
| $v_0$ | 96 m/d | $r_h$ | 0.00019 $m^3/g$ |
| $v_{00}$ | 80 m/d | $r_p$ | 0.0007 $m^3/g$ |
| $f_{ns}$ | 0.24 | | |



evaluated by calculating the average relative deviation (ARD) between model predictions and available data points for the parameter set resulting from the parameter fitting procedure (Eq. 2):

$$\mathrm{ARD} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{\left|Xi_{\mathrm{obs}} - Xi_{\mathrm{sim}}\right|}{Xi_{\mathrm{obs}}}\right)\times 100\% \qquad (2)$$

where:

ARD = average relative deviation;

$n$ = number of experimental data points;

$Xi_{\mathrm{obs}}$ = observed values;

$Xi_{\mathrm{sim}}$ = simulated values.

## Results and discussion

### Reference simulation

A simulation with the original WEST Takacs model was first done and served as a reference simulation. The model fit is reasonably good for $COD_X$ concentrations (Figure 1) with an ARD of 31%. However, it could be improved as, on the average, there seems to be an underestimation of the $COD_X$ concentration, while peaks are overestimated (e.g. day 9 and 10). Effluent $COD_S$ concentrations (Figure 2) are slightly overestimated (ARD of 21%), indicating a net loss of $COD_S$ in the clarifier. Moreover, changes in simulated effluent $COD_S$ are too sudden and too big compared to the changes of the measured values. This last point can be explained because the influent soluble components are immediately passed on to the effluent in the original WEST Takacs model implementation. Thus, soluble

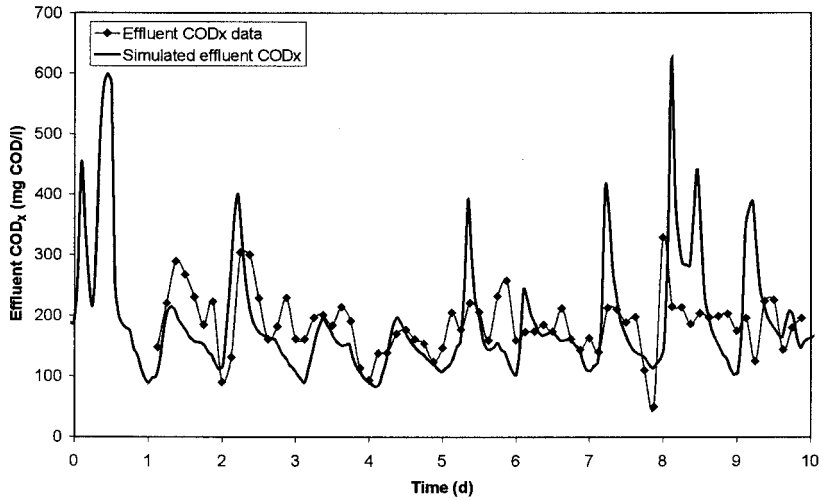


**Figure 1** Original Takacs model; model fit for simulated effluent $COD_X$ concentration

**Table 2** Results of Takacs settling parameter estimation for the original WEST Takacs model

| Settling parameter set 1 | Value | Variable | ARD (%) |
|---|---|---|---|
| $v_0$ | 199.805 m/d | Effluent $S_S$ | 18.4 |
| $v_{00}$ | 31.256 m/d | Effluent $COD_X$ | 22.4 |
| $r_p$ | 1.328e–4 $m^3/g$ | Effluent $COD_S$ | 21.8 |
| $r_h$ | 1.006e–6 $m^3/g$ | Effluent $S_{NH}$ | 12.5 |
| $f_{ns}$ | 1.089e–5 | | |
| **Settling parameter set 2** | **Value** | **Variable** | **ARD (%)** |
| $v_0$ | 250 m/d | Effluent $S_S$ | 18.4 |
| $v_{00}$ | 240 m/d | Effluent $COD_X$ | 22.3 |
| $r_p$ | 1.064e–4 $m^3/g$ | Effluent $COD_S$ | 21.8 |
| $r_h$ | 1.183e–6 $m^3/g$ | Effluent $S_{NH}$ | 12.5 |
| $f_{ns}$ | 1.003e–5 | | |

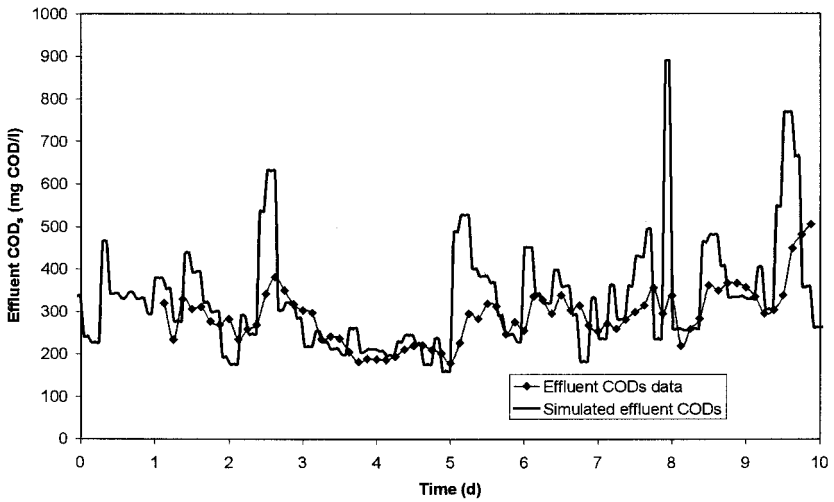


**Figure 2** Original Takacs model; model fit for simulated effluent $COD_S$ concentration

components do not have a residence time in the clarifier (with some mixing) and the effluent concentration changes follow the drastic influent concentration changes.

#### Estimation of settling parameters based on effluent $COD_X$

Tests were made to improve the model fit by estimating new settling parameters ($v_0$, $v_{00}$, $r_p$, $r_h$ and $f_{ns}$) which were adjusted in order to get an optimal fit on effluent $X_I$ data. For $X_I$, identical fractions were applied for the effluent and influent data ($X_I$= 0.2 $COD_X$). By doing this it was in fact assumed that the settler does not alter the ratio between the different fractions of particulate material: no reactions take place in the Takacs settler and all particulate fractions settle with the same velocity.

It appeared that estimation of Takacs settling parameters based on $COD_X$ data in the overflow is far from straightforward. Indeed, it was observed that the model fit increased only slightly for rather big parameter variations (especially $v_0$). This parameter identifiability problem leads to different parameter combinations that resulted in almost identical model fits (Table 2).

The Takacs settling curves for both sets of Takacs settling parameters resulting from the parameter estimations (see Table 2) were plotted (Figure 3). The two settling curves of Figure 3 are completely different, indicating that there is a parameter identifiability

**Table 3** Relative sensitivity of model output (SS concentration in layer 1 and 10 of the primary clarifier) for the Takacs settling parameters and the design parameters $A$, $H$ and $Q_u$

| Parameter | $X(1)$ | Sensitivity | $X(10)$ | Sensitivity |
|---|---|---|---|---|
| $A$ | –0.5133 | *** | 0.2462 | ** |
| $H$ | 0.0348 | * | 0.0017 | * |
| $Q_u$ | –0.0136 | * | –0.9609 | *** |
| $v_0$ | –0.5464 | *** | 0.2445 | ** |
| $v_{00}$ | 0.0000 | – | 0.0000 | – |
| $r_p$ | –0.7193 | *** | 0.3108 | ** |
| $r_h$ | 0.2136 | ** | –0.1324 | ** |
| $f_{ns}$ | 0.3816 | ** | –0.2230 | ** |

N.B. – = not sensitive; * = slightly sensitive; ** = moderately sensitive; *** = very sensitive

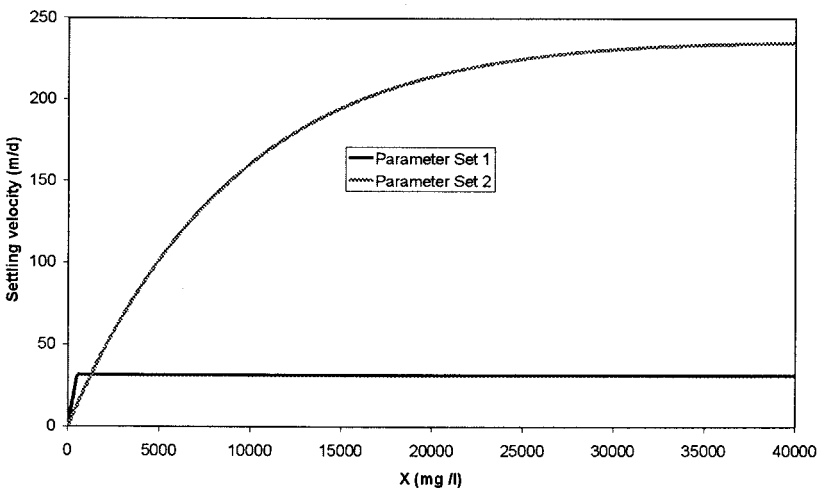


**Figure 3** Takacs settling curves for parameter set 1 and 2 resulting from the parameter estimation procedure

problem with respect to estimating Takacs settling parameters when only overflow $COD_X$ concentration values are available. It was finally tried to estimate the Takacs settling parameters $v_0$, $v_{00}$, $r_p$, $r_h$ based on overflow $COD_X$ concentrations, while the Takacs settling parameter fns was fixed at a value of 0.25. That value is similar to the $f_{ns}$ value obtained by Coderre (1999) and represents a more realistic ratio of non-settleable/settleable solids. However this modification of the estimation procedure did not lead to improved parameter identifiability.

#### Sensitivity of Takacs model output to changes in settling and design parameters

Due to this identifiability problem, the sensitivity of the Takacs model output to model parameter changes was tested. Relative sensitivity functions were calculated based on the difference between the model output obtained for a reference set of parameters and the model output obtained by increasing the value of one parameter with 0.5% (see Eq. 3). This procedure was repeated for all settling parameters ($v_0$, $v_{00}$, $r_p$, $r_h$ and $f_{ns}$) and for the primary clarifier design variables (surface $A$, height $H$, underflow flow rate $Q_u$). The Takacs settling parameters of Coderre (1999) were used to generate the reference simulation.

$$f = \frac{dy}{y}\frac{\theta}{d\theta} \tag{3}$$

where $f$ = value of relative sensitivity function; $dy$ = model output difference; $y$ = reference model output (for reference parameter set); $d\theta$ = parameter difference; $\theta$ = reference value of parameter.

The results of this evaluation are shown in Table 3. The evaluation was done for $X(1)$ and $X(10)$, the SS concentration in the top and the bottom layer of the clarifier respectively. It is surprising that the model output was not sensitive at all to variations of the settling parameter $v_{00}$.



#### Estimation of settling parameters based on effluent $COD_X$ and underflow SS

It was also tried to estimate the settling parameters using both the overflow $COD_X$ and the underflow SS concentrations (no underflow COD data available). One of the reasons to set up the parameter estimation procedure like this was the poor description of the underflow SS concentration data when only fitting on overflow $COD_X$ data.

Multivariable fitting on both overflow and underflow SS concentrations did not give satisfactory results. When using the settling parameters resulting from the parameter estimation procedure in a simulation, it appeared that a reasonable description of underflow SS concentrations could be achieved. However, too few solids went to the overflow, resulting in predicted overflow SS concentrations that were far too low. The explanation is the huge difference between the overflow and underflow SS concentration. For multivariable fitting the underflow SS concentrations will weigh much more compared to the overflow concentrations, since the optimization procedure relied on the minimization of the absolute sum of squared errors between model predictions and available data.

A possible solution to fit the model correctly on both data sets is the application of weighting factors on the different available data sets. A weighting factor of 0.001 was applied for the underflow SS data, and a factor 1 was used for overflow $COD_X$ data. By doing this, the fit on underflow SS data became worse whereas the fit on overflow $COD_X$ improved. Still, model fit on overflow $COD_X$ was not sufficiently good.

A more fundamental explanation for the problems found could be the choice of a proper COD/SS ratio in the Takacs model. Indeed, since it was attempted to have an ASM1 compatible settler model, the influent concentrations were all expressed in terms of COD concentrations. Particulate COD concentrations need to be converted into SS units for the calculation of the settling velocity of the SS in the settler. It was observed from the data that the $COD_X$ /SS ratio in the influent (0.91) is different from the $COD_X$ /SS ratio in the overflow (1.22) of the primary clarifier. For the underflow data this could not be checked since no COD data were available. For the original Takacs model this creates a problem, since one can only apply one COD to SS conversion factor in the model. The observed variation of the $COD_X$ /SS fractions can be caused either by the fact that different particulate fractions do not settle with identical velocities, or by the production or consumption of certain particulate fractions during the residence time in the primary clarifier. Production or consumption of particulate fractions in the clarifier could be modelled by adding reactions to the Takacs clarifier model, as will be illustrated below, and could for example account for the extra formation of some SS through flocculation of $COD_S$ fractions.

#### Takacs model with soluble residence time and flocculation of $COD_S$

As a start, a new model was built where the transport and mixing of the soluble components was assumed to be due to the bulk movement of the liquid. The soluble components are passed on through the different layers of the Takacs clarifier as though they were passing through tanks in series. Results of simulations are given in Figure 4 for effluent $COD_S$. The modified model gave a better fit for effluent $COD_S$ compared to the original Takacs model (Figure 2) (ARD = 18.9% compared to 21.8%). From Figure 4 one can observe that the

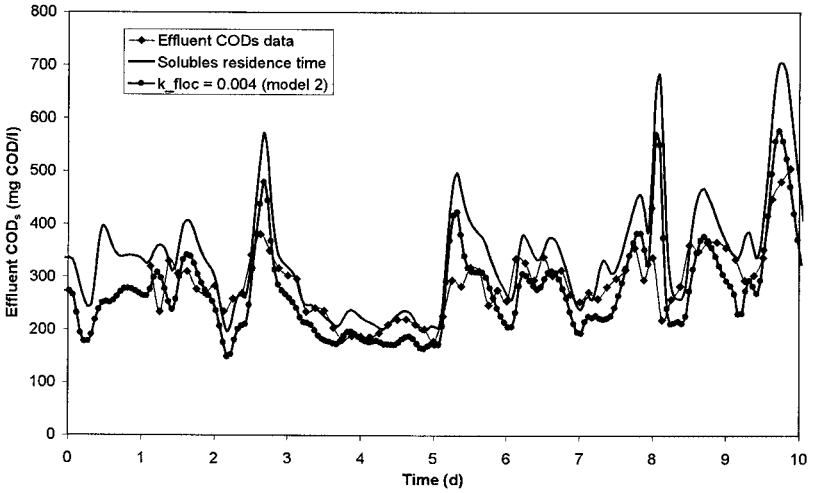


**Figure 4** Simulated effluent $COD_S$ concentration for Takacs model with solubles residence time and Takacs model with flocculation reaction (k_floc = 0.004; flocculation model 2)

simulated effluent $COD_S$ concentrations are on average still higher than the measured ones.

As mentioned before, a net loss of soluble COD was observed in the primary clarifiers of the Norwich WWTP. It was thus assumed that this loss was due to flocculation of soluble COD and that both $S_S$ and $S_I$ were removed partially through this phenomenon. The flocculation rate was first assumed to be a first order reaction (e.g. flocculation rate = k_floc SI). The constant k_floc was assumed to be the same for $S_I$ and $S_S$. During the flocculation process, $S_I$ was converted to $X_I$, and $S_S$ was converted to $X_S$. It was also considered to include hydrolysis in the model (conversion of $X_S$ to $S_S$), but from a model calibration point of view this has no meaning in this particular case. Indeed, hydrolysis of $X_S$ to $S_S$ can always be compensated by flocculation of $S_S$ to $X_S$, which means that the flocculation and hydrolysis rate will be highly correlated. It should be clear however that it can be interesting to include a hydrolysis reaction in the settler model, especially in case measured effluent $COD_S$ concentrations are higher than influent $COD_S$ concentrations (net production of $COD_S$ in the primary clarifier).

The model fit on $COD_S$ data was first improved by estimating the value of k_floc that resulted in the best description of effluent $COD_S$ data; a k_floc value of 1.249 $d^{-1}$ was obtained. An average relative deviation between model predictions and measured $COD_S$ values of 15.1% was calculated. This is a significant improvement in comparison with previous simulations with the original Takacs model (21.8%) and the Takacs model with soluble residence time (18.9%).

Following this study, a second model was developed where the flocculation rate of $S_I$ or $S_S$ was dependent both on the $S_I$ or $S_S$ concentration and the total $S_S$ concentration (e.g. flocculation rate = k_floc $S_I$ $X$). The flocculation rate constant k_floc was again assumed to be the same for $S_I$ and $S_S$. During the flocculation process $S_I$ was converted to $X_I$, and $S_S$ was converted to $X_S$. For this flocculation model, k_floc cannot be estimated independently from the settling parameters when trying to optimize the model fit on effluent $COD_S$ data. Indeed, in this second flocculation model the amount of flocculated $S_I$ or $S_S$ will also depend on the $S_S$ concentration in the layers. A modification of the settling parameters will thus also result in a modification of the amount of $S_I$ and $S_S$ that will be converted to $X_I$ and $X_S$ through flocculation.

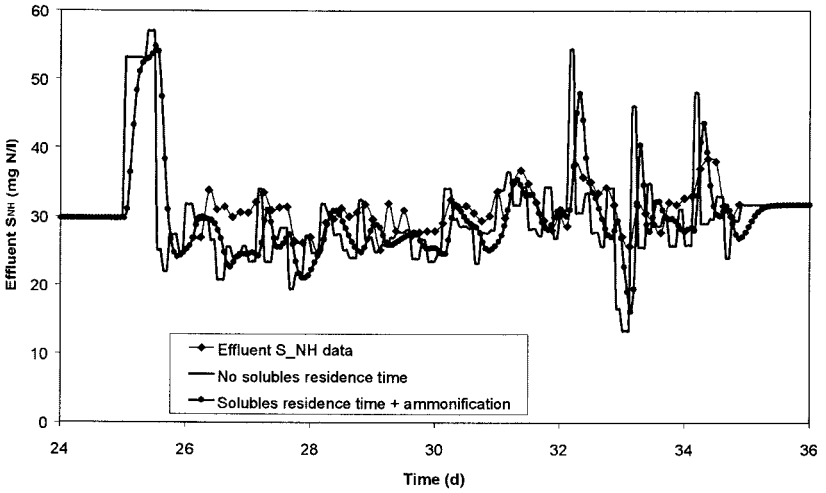


**Figure 5** Model fit to effluent $S_{NH}$ data for Takacs model without solubles residence time, and for a Takacs model with solubles residence time and ammonification (k_a = 1.49 1/d)

However, in a first approximation k_floc was estimated separately. The value obtained from this estimation (k_floc = 0.0047 l/mg COD.d) was subsequently used as the initial value for a second optimization run in which both settling parameters and k_floc were estimated. A new parameter estimation was carried out to estimate k_floc and the settling parameters. Effluent $COD_S$ and $COD_X$ data were used as fit criteria (multivariable fitting). A k_floc value of 0.0040 l/mg COD.d resulted from the estimation procedure together with a set of settling parameters. A simulation was carried out using the parameter set resulting from the estimation procedure. An average relative deviation between model predictions and measured $COD_S$ values of 15.2% was obtained, similar to the first flocculation model. The model fit is also shown in Figure 4. The model fit to effluent $COD_S$ data obtained for this second flocculation model is slightly worse compared to the first model (15.2 versus 15.1% average relative deviation respectively). Obviously, the less complex model is to be preferred since the extra complexity introduced by using flocculation model 2 did not improve the results.

#### Takacs model with ammonification

For the original Takacs model implementation in WEST, an average relative deviation between model predictions and data of 12.5% was found. Similar to $COD_S$ data, concentration changes predicted by the model were too sudden and too sharp (see Figure 5). In a first phase, the model fit on effluent $S_{NH}$ data improved by including the solubles residence time in the Takacs model, with a resulting ARD value of 10.2%. It was then tried to improve the model fit by including ammonification in the model. In the ammonification process influent $S_{ND}$ is converted to $S_{NH}$. Ammonification was included in the model as $r_{amm} = k\_a\, S_{ND}$. The value of k_a was estimated in order to get the best fit on effluent SNH data. A value of 1.49 1/d was obtained for k_a, and an average relative deviation between model predictions and measured $S_{NH}$ values of 8.6% was calculated. The resulting model fit on $S_{NH}$ effluent data is also shown in Figure 5.

## Conclusions

A Takacs settler model can give a reasonable description of the effluent $COD_X$ concentrations of a primary clarifier. However, it became clear from the parameter estimations that

effluent $COD_X$ or SS concentrations are not sufficient to make the settling parameters identifiable since several sets of parameters could be found that resulted in similar model fits. A possible solution to improve model identifiability is a multivariable fitting procedure that uses the underflow SS concentrations as a second information source. However, to have an adequate description of both overflow and underflow SS one should apply weighting factors on the data sets, since the contribution of the underflow SS concentration to the sum of squared errors fit criterion will be significantly higher compared to overflow concentrations (the concentrations are about 100 to 1000 times higher in the underflow). Even then it is difficult to achieve good model fits on both underflow and overflow data because COD conversion reactions in the primary clarifier might alter the COD/SS ratio of the particulate material that enters the settler, as could be observed from the available data.

For soluble components ($COD_S$, $S_{NH}$), including a soluble residence time in the Takacs clarifier model resulted in a much better description of effluent soluble components concentrations. In addition, $COD_S$ concentrations were more accurately described when a flocculation term (conversion of $S_I$ to $X_I$ and $S_S$ to $X_S$) was added to the Takacs model. Two flocculation models were tested. In the first model flocculation of $S_I$ and $S_S$ was only depending on the $S_I$ and $S_S$ concentration. In the second model flocculation was also depending on the total SS concentration in the layers. Both models resulted in a similar improvement of the model fit to effluent $COD_S$ data. For practical applications the first model is to be preferred since its calibration is easier compared to the second flocculation model. Including an ammonification reaction in the primary clarifier further improved the model fit on effluent $S_{NH}$ data.



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