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RESEARCH ARTICLE

Calibration and validation of a dynamic model for water quality in combined sewer retention tanks

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As the integrated management of urban wastewater systems becomes more and more popular, the development of wastewater management subsystem models appears essential to improve the understanding of the pollutant dynamics and their interactions. In such a context, a review of the literature reveals a lack of efficient models describing the dynamics of the water quality stored in off-line retention tanks. A model has thus been proposed based on the fractionation of suspended solids into three classes according to the particle settling velocity distribution measured in the field using the ViCAs settling test. In this paper, a calibration methodology is developed and full-scale field data sets from three different events are used for 1) calibrating this new dynamic retention tank model (two data sets); and 2) validating that model on the last data set. The results show a good agreement between observed and simulated data both for the total suspended solids and the total chemical oxygen demand.

Keywords: combined sewer overflow; settling velocity; stormwater management; urban wastewater modelling; water quality; wet weather

1. Introduction

To improve operation of combined sewer overflow retention tanks (RT), important infrastructures for urban stormwater management, it is necessary to consider the system as a whole (Rauch *et al.* 2002), following the fate of water from catchment runoff down to the receiving body. The scale of such a system is so big that it becomes rather difficult to assess the interactions between the different subsystems with *in situ* measurements. In such a context, modelling appears a very useful tool as the phenomena occurring in RTs are increasingly understood. To feed a new modelling approach, Maruéjouls *et al.* (2011) suggest a sampling protocol that allows a proper quantification of the main processes driving water quality in RTs such as settling and resuspension. For the studied RT, the total suspended solids (TSS) and total chemical oxygen demand (CODt) concentrations observed at the outlet show a 'U' shape, distinguishing three phases:

- An initial pollutant peak that lasts around 15 minutes. This concentration peak is the result of particle resuspension in the pumping well due to the pumps' activation for emptying. The observations reported that an average of 23% of particles is sent to the wastewater treatment plant (WWTP) during this phase (average made over seven events).
- A middle phase that is characterized by an ongoing concentration decrease due to settling. The average concentration is quite low, i.e. around 93 g/m^3 (average made over 15 events).
- The final peak in particle concentration is due to particle resuspension as a result of the small volume of water that remains in the tank at the end of emptying, increasing shear stress. The average of the fraction of mass of particles emptied during this phase is around 13 % (average made over seven events).

These features are also confirmed by results of a phenomenological model built on the basis of these observed phenomena. The simulation results were shown to fit full-scale field data in Maruéjouls *et al.* (2012).

Modelling the dynamics of the water quality that is stored in sewers and specifically in RTs, can help improving the accuracy of the predictions of WWTP influent quality. One of the important elements that stand in the way of integrated modelling improvements is the compatibility between the submodels in terms of state variables and parameters (Fronteau *et al.* 1997, Rauch *et al.* 2002). When developing new models, it is thus necessary to consider the parameters and variables of the models to which they will be linked. Also, the new models need to: 1) be tested with full-scale data, 2) be compatible with one another and 3) require only a short calculation time.

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The first approach for RT modelling is computational fluid dynamics (CFD) models, e.g. Vazquez *et al.* (2008). However, the long calculation times do not allow their use in an integrated system context. A different approach investigated in this study is more phenomenological in nature and requires considerably fewer calculations. Most of such RT models available today are quite simple as they consist of linear reservoirs representing the hydraulics and not paying a lot of attention to the water quality dynamics. However, several modelling studies taking into account water quality have already been carried out. They describe the settling processes in a more or less complex way. Some use a single removal rate value in a set of ordinary differential equations (Lessard and Beck 1991, Wong and Geiger 1997) and/or an average settling velocity (Vs) parameter (Frehmann *et al.* 2005, Kutzner *et al.* 2007) and/or surface load as predominant factor (Vaes and Berlamont 1999, Luyckx *et al.* 2002) while some others add different operational modes distinguishing pollutant behaviour for filling, overflow, storage or emptying phases (Lessard and Beck 1991). Nevertheless, none of these models has ever been successfully validated with full-scale field data (Kutzner *et al.* 2007).

Particle settling velocity distribution (PSVD) studies on such infrastructures are quite rare, but many authors agree on the relevance of such characteristics (Michelbach 1995, Boxall *et al.* 2007, Maruéjouls *et al.* 2012). Even if a the meaning of a settling velocity can be easily understood from a physical point of view, determining an average Vs value describing the whole settling processes is a difficult task as particle Vs, and even PSVD, found in combined sewers are known to vary a lot (Michelbach 1995, Maruéjouls *et al.* 2011). As an incentive to this study, Vallet *et al.* (2013) already proved the potential and interest of using classes of particles with different Vs for settling modelling in stormwater basins.

The current work presents the calibration method of a new off-line RT dynamic model based on the Maruéjouls *et al.* (2012) model. The new model describes sedimentation, resuspension and hydrolysis processes using three different particle classes associated with three different Vs. The first part of this paper describes the methodology used for the calibration. The second part shows simulation results obtained during the calibration and validation.

2. Material and methods

2.1. The data

The data used for the calibration and the validation presented in this study come from two sampling campaigns performed during the summers 2009 and 2010 on a 7580 m^3 off-line RT located on a combined sewer in Quebec City, Canada. The whole sampling and analysis methodology is more detailed in Maruéjouls *et al.* (2011).

The measurement of settling characteristics was carried out with the ViCAs test (Chebbo and Gromaire 2009). This protocol uses a 2.5 L plexiglas column in which the wastewater sample is introduced rapidly and maintained thanks to a vacuum. At various time steps, settled particles are collected at the bottom of the column and weighed. A small numerical treatment of the data is then used to find the PSVD fitting the collected accumulated mass.

2.2. The retention tank model

The developed model represents the mechanisms driving pollutant behaviour occurring in the system by using ordinary differential equations. It is a 1-D dynamic off-line RT model using ordinary differential equations inspired by Lessard and Beck (1991). The main improvements are adding a pumping well (PW) and changing the settling model using three particle classes associated with three Vs. A more accurate description of the whole concept of the model is detailed in Maruéjouls *et al.* (2012). A scheme of the included processes is presented in Figure 2. The ultimate goal of such a model is its integration in a 'combined sewer – WWTP' model. The pollutant behaviours (TSS and CODt) are mainly reproduced through two processes, the settling and the resuspension of particles. The ViCAs tests give a PSVD, summarised for the model in three particle classes representing: 1) a fraction with a very low Vs where the largest part will never settle during storage (variables marked 1); 2) a fraction settling more slowly for which it takes many hours to be completely removed (variables marked 2) and 3) a particle fraction that settles quickly when entering the tank (variables marked 3). The model includes a fractionation step for both TSS and CODt variables as shown in Figure 1. Such a fractionation makes the model compatible with activated sludge models using ASM1 (Henze *et al.* 1987) variables. Indeed, CODt fractionation is based on the ASM1 fractionation concept since CODt is split in a particulate (*X*) and soluble (*S*) fraction which are further split in biodegradable (*Xs*, *Ss*) and inert (*Xi, Si*) fractions. Then, particulate variables(*TSS*, *Xs*, *Xi*) are fractionated in particulate classes where the number (1, 2 or 3) refers to a specific Vs. Further fractionation into ASM1 fractions are not discussed in detail. They come from a number of respirometry analyses performed on RT wastewaters and fractionation values found in the literature.

As shown in Figure 2, the retention tank model includes settling ($Sett_j$) and resuspension (R_{RTj}) processes between two layers (*Clar* and *Sludge*) for each particle class (*j*). Resuspension in the tank happens when the pumps are running and only a small volume of wastewater is still in the tank increasing shear stress. Water fluxes that convey particulate and soluble pollutants are represented by *Jj*. The same processes are implemented in the pumping well but for three layers ('*Up*', '*Mix*' and '*Down*'). $J_{1,j}$

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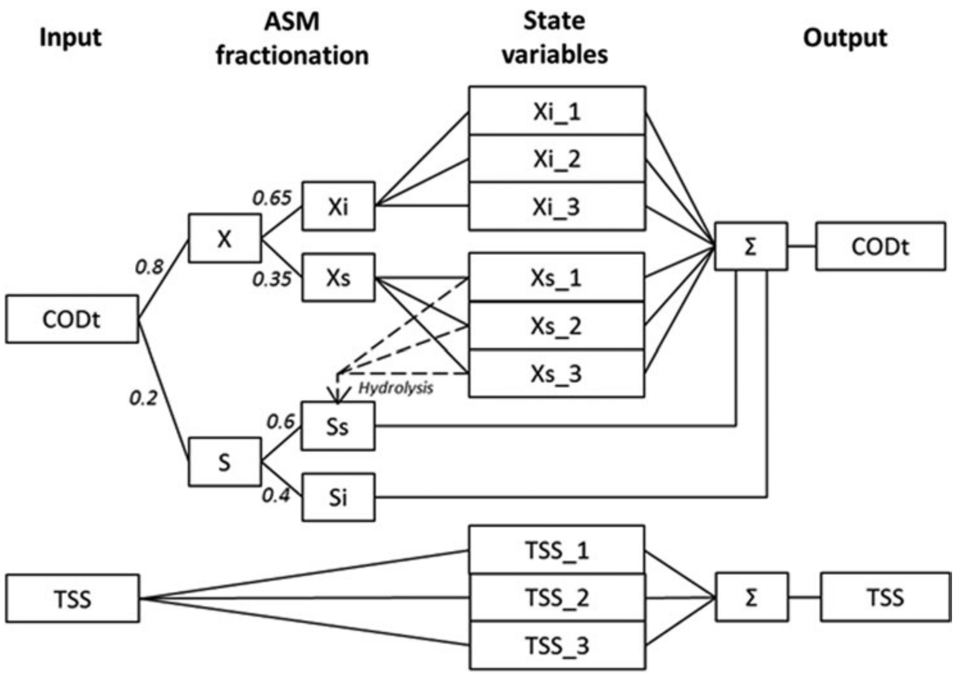

Figure 1. Fractionation concept of the collected data (input) to the model variables. Variables named Xx_1,2,3 are subject to sedimentation/resuspension. Subscripts 1, 2 and 3 refer to specific particle classes and settling velocities. Hydrolysis reactions occur between Xs_1,2,3 and Ss variables.

represents fluxes between layers '*Up*' and 'Mix' and $J_{2,j}$ represents fluxes between layers '*Mix*' and '*Down*'. These three layers allow particles contained in layer '*Down*' to be resuspended in layer '*Mix*' when pumps are activated and not in layer '*Up*'. The model output is the result of the $J_{Down,i}$ flux going out of layer '*Down*'. Figure 2 presents the concept of the model proposed by Maruéjouls *et al.* (2012) that was improved in three ways:

- A fourth accumulation layer was added in the pumping well (in grey) in order to trap a particle fraction which won't be resuspended and will remain in that layer until a manual extraction.
- The description of the output quality/quantity is solely described by the $J_{Down,j}$ flux which is coming out from the '*Down*' layer and has the same water quality.

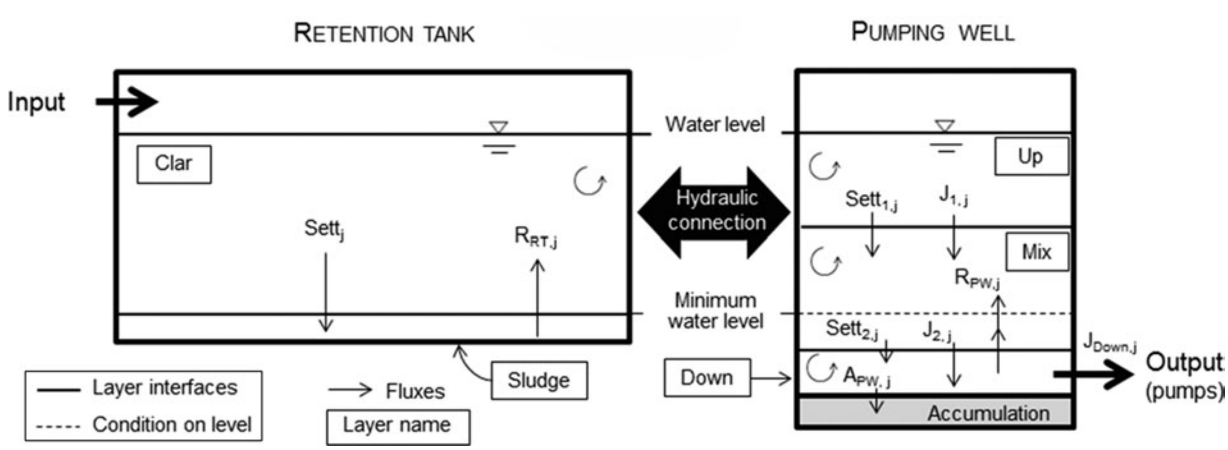

Figure 2. RT/PW model conceptual diagram from Maruéjouls *et al.*, (2012) improved in three ways (see text).

- A hydrolysis process was added allowing the transformation of particulate biodegradable matter (*Xs_1,2,3*) in soluble biodegradable matter (*Ss*). Since it was shown that the organic matter biodegradability is heterogeneously distributed with respect to the particle Vs (Hvitved-Jacobsen *et al.* 1998), three different rates are available depending on the Vs class.

2.3. The calibration method

The calibration of the thirteen parameters is roughly made up of three main steps, see Figure 3. The first stage is represented by the continuous line until the Vs fractionation step 1 calibration is completed. Then, the second stage is illustrated by the dotted line. The Vs fractionation steps are found to be the most tedious task and will be further detailed.

2.3.1. Pumping well (PW) layer volumes, resuspension rates and the sludge accumulation

The calibration of these parameters is subject to an iteration aiming at an optimization before going to the next step. The volumes, V_{Min}, V_{Mix} and V_{Down} (in m^3), are fitted to the effluent quality during the first 20 minutes of emptying. Indeed, the essential purpose of those three volumes is the distribution of the resuspended particles in the bulk due to the pumps' activation. This phenomenon is visible on the emptying pollutograph of those first minutes. After that, all resuspended particles are extracted. Thus, the shape of the first peak highly depends on PW volumes. For example, if the '*Down*' volume is too small, the particles would be extracted too fast. The resuspension rate (in h^{-1}) in the PW (R_{PW}) is calibrated by fitting on the same data and is also important for model performance, i. e. when that rate is too slow, the particles are not resuspended enough and are thus extracted too fast. For resuspension in the RT, R_{RT} is calibrated with regards to the pollutant concentration observed during the last ten minutes of emptying. Indeed, the increasing load at the end of emptying is due to the resuspension of particles accumulated at the bottom of the retention tank. Finally, sludge accumulation, A_{PW} (in %), is calibrated by fitting the mass of particles that has accumulated at the bottom of the PW as observed in the field. Before moving on to the next step (hydrolysis kinetics), a final iteration is performed.

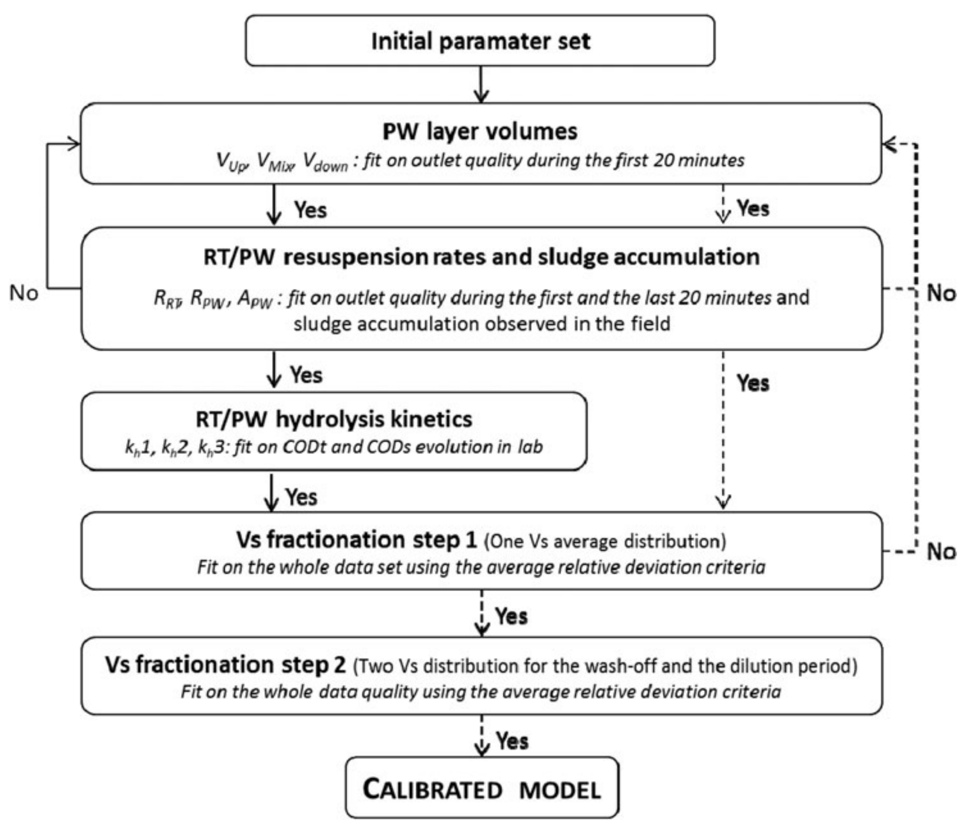

Figure 3. Model parameter calibration steps. The first path to follow is represented by the continuous line and the second path by the dotted line.

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2.3.2. *The hydrolysis kinetics*

Including the hydrolysis process allows transforming a fraction of the *Xs1*, *Xs2* and *Xs3* into soluble biodegradable COD (*Ss*), according to a first order hydrolysis model (Equation (1)). The hydrolysis rates, k_{h1}, k_{h2} and k_{h3} (in h^{-1}) corresponding respectively to class 1, 2 and 3, were calibrated by fitting laboratory experimental results. The experiment to be conducted consists in measuring the evolution of the total and soluble COD in a wastewater sample from the tank. This sample is inserted in a beaker and left settling for 24 hours in order to reproduce the storage conditions occurring in the tank. The measurements are collected in the middle of the beaker with a piston-driven air displacement pipette. The optimal k_h value found is then used for k_{h1}, k_{h2} and k_{h3}.

$$S(t) = Si_o + Ss_o + Xs_o(1 - e^{-k_h \cdot t}) \qquad (1)$$

S(t), Soluble COD concentration (g/m^3); Si_o, Initial inert soluble COD concentration (g/m^3); Ss_o, Initial biodegradable soluble COD concentration (g/m^3); Xs_o, Initial biodegradable particulate COD concentration (g/m^3); k_h, Hydrolysis rate (h^{-1}); t, Time (h).

2.3.3. *Vs fractionation*

Based on an approach proposed by Vallet *et al.* (2013)who developed a model for stormwater tanks in separate sewers the Vs fractionation starts from measurements carried out using the ViCAs protocol. The Vs fractionation methodology consists in two steps that are further detailed below. The different Vs combinations tested and average relative deviation (ARD, Equation (2)) performance results are detailed here in Figure 6.

$$ARD = \frac{\sum_{i=1}^{n}(|x_{obs} - x_{sim}|/|x_{obs}|)}{n} \cdot 100 \qquad (2)$$

ARD, Average relative deviation (%); x_{obs}, Observed pollutant concentration (g/m^3); x_{sim}, Simulated pollutant concentration (g/m^3); n, Number of observed values.

2.3.3.1. *First step (one ViCAs).* To illustrate this calibration step, particle Vs distributions from the influent samples are presented in Figure 4. The dashed curve (Figure 4(a)) is an average made over all ViCAs results collected at the studied RT (ten data sets). The first step of the calibration is performed by moving the class limits (dotted lines) over that average curve until the simulated TSS and CODt concentration results fit the measured concentrations in the outlet during emptying (see Figures 7 and 8). The Vs assigned to those classes are found by calculating the geometric average on the abscissa between the boundaries. For example, the limits drawn on Figure 4 correspond to: class 1 = 20% of the total particle mass with a *Vs1* = 0.035m/h; class 2 = 30% with a *Vs2* = 0.4 m/h; and class 3 = 50% with a *Vs3* = 4.8 m/h. Once the class limits are defined, the ViCAs curve gives the TSS fractions belonging to each of the three classes. Therefore those are no longer considered model parameters to be fitted.

2.3.3.2. *Second step (two ViCAs).* On Figure 4(b), two ViCAs curves corresponding to two different wastewater types are distinguished. Indeed, Maruéjouls *et al.* (2011) observed a possible correlation between TSS concen-

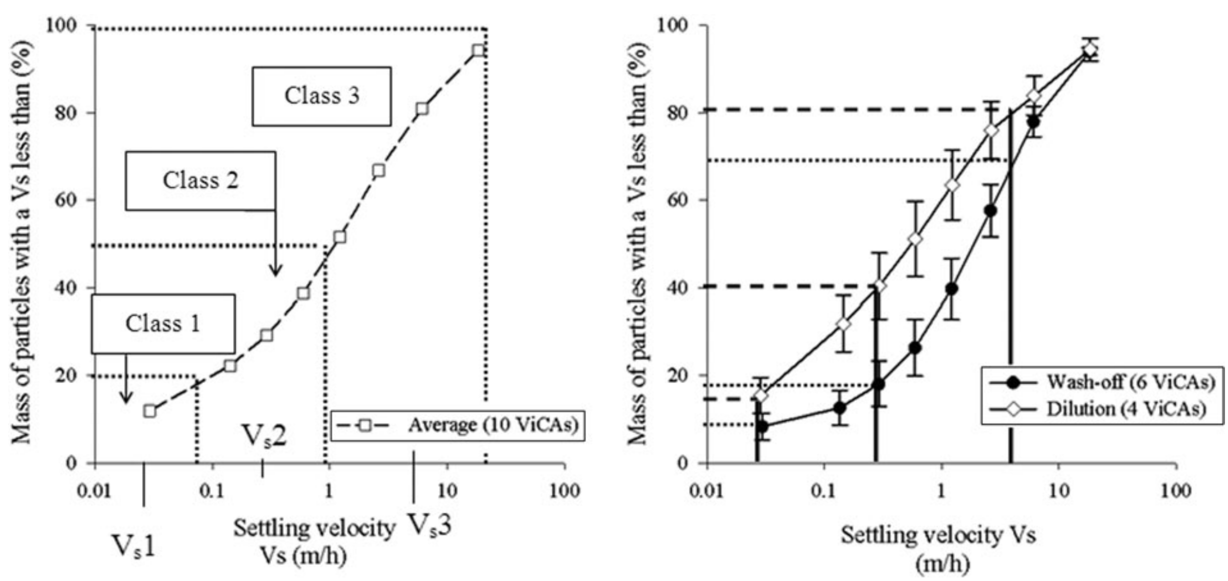

Figure 4. Vs fractionation description for the three classes' definition. a) Calibration on one ViCAs average, b) Vs distributions used for calibration on two ViCAs averages ('Wash-off' and 'Dilution' periods).

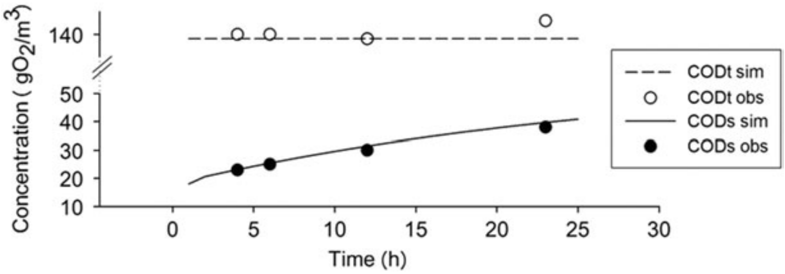

Figure 5. Calibration results of the hydrolysis rate.

tration and Vs distribution. The '*Wash-off*' curve is an average of ViCAs results obtained over six samples collected during the first flush (Bertrand-Krajewski *et al.* 1998, Deletic 1998). Typically, that period corresponds to high TSS concentrations. The '*Dilution*' curve is an average of ViCAs results from four samples collected during the period which comes after the '*Wash-off*', i.e. when wastewater is diluted with stormwater. The second step of the Vs fractionation calibration is performed using those two curves.

The four Vs values obtained with the ViCAs average PSVD that gives the lowest ARD are then used as a starting point to find the limits of the classes within both the '*Wash-off*' and '*Dilution*' period. On Figure 4(b) the two different ViCAs are shown with their peculiar TSS fractionation, i.e. three classes for the '*Wash-off*' period and three others for the '*Dilution*' period. The TSS concentration value separating the two periods is a new parameter to set. Maruéjouls *et al.* (2012) set this threshold value to 100 g/m^3 on the basis of measurement results showing that the '*wash-off*' period ends when the TSS concentration reaches approximately 100 g/m^3. Tuning this parameter mainly impacts the '*middle*' phase. This impact is bigger when the event is small. For instance, when the parameter is set to 1500 g/m^3, particles settle slower resulting in a shift upward of the average concentrations of the '*middle*' phase (around 80 g/m^3 more) for short filling and retention times. For longer filling and retention times, the sensitivity is lower due to the fact that particles have time to settle to a large extent even with low settling velocities. Again, this calibration method makes that the TSS fractions are directly defined by the Vs class limits, i.e. a unique fraction corresponds to a unique Vs for each ViCAs.

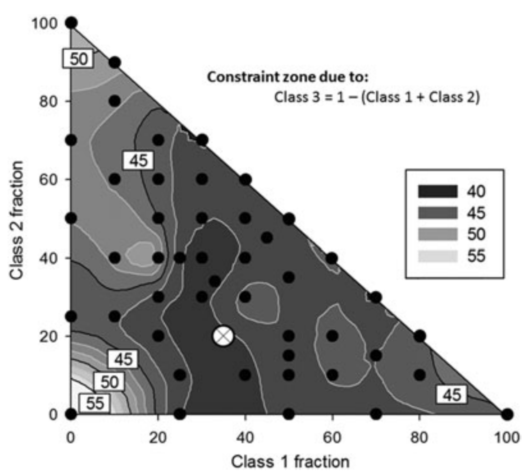

Figure 6. Average relative deviation results of Vs fractionation calibration step 1. ARD areas are an average of four ARD values which are obtained for TSS, CODt for two simulated events. The points correspond to the fractionation parameter values used for calibration. The white point represents the equivalent at step 1 of the final calibrated values found at step 2.

Once the calibration of the Vs fractionation is finalised, iteration is carried out to optimise the PW volumes, the resuspension and the sludge accumulation rates. Then, after a last Vs fractionation step, the model is considered calibrated.

3. Results and discussion

In the next paragraph, the chosen parameter values and the pollutographs resulting from the calibration and validation steps are presented and discussed. Two different events were used for the calibration in order to avoid event dependent parameter values. The last event was kept for the validation step which consists in running a simulation without tuning any parameter.

3.1. Calibration

3.1.1. Hydrolysis rates

Results of the hydrolysis rates calibration (k_{h1}, k_{h2}, k_{h3}) are reported in Figure 5. The laboratory experiments reveal a quite constant CODt and a slightly increasing soluble COD, around 1g/m^3/h. That means that a fraction of the particulate COD is transformed in soluble COD. In the current study, the hydrolysis rate is important enough to be noticeable in laboratory tests. Nevertheless, in the current simulations the simulation outputs are quite insensitive to their value. The calibration was performed using the CODt and soluble COD results of a laboratory experiment.

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Table 1. Parameter values resulting from the calibration. Shaded zones indicate parameters that are obtained from lab experiments.

Parameters		Calibrated values
PW layer volumes	$V_{Min}(m^3)$	13
	$V_{Mix}(m^3)$	40
	$V_{Down}(m^3)$	11
Resuspension rates	R_{PW} (h^{-1})	41
	R_{RT} (h^{-1})	41
Accumulation	A_{PW} (%)	50
Settling velocities	*Vs1 (m/h)*	*0.08*
	Vs2 (m/h)	*1*
	Vs3 (m/h)	*6*
Wash-off/Dilution TSS limit	*Lim*(g/m^3)	*100*
Hydrolysis rates	k_h1 (h^{-1})	*0.035*
	k_h2 (h^{-1})	*0.035*
	k_h3 (h^{-1})	*0.035*
Fraction wash-off	f_w1 **(%)**	***30***
	f_w2 **(%)**	***15***
	f_w3 **(%)**	***55***
Fraction dilution	f_d1 **(%)**	***55***
	f_d2 **(%)**	***15***
	f_d3 **(%)**	***30***

3.1.2. *Vs fractionation calibration steps*

Using the scenario analysis mode provided by WEST, around fifty PSVD parameter combinations for the Vs fractionation were tested (Figure 6). After this calibration, no further iteration with PW volumes or resuspension rates had to be performed. For every Vs combination tested the ARD was calculated in order to find the optimal combination. Each ARD value plotted on Figure 6 is an average of four ARD values calculated for TSS and CODt over two events. Abscissa and ordinate axes represents values of TSS fraction 1 and 2 for each combination. Since the fraction of class 3 is dependent on the two others, the space of Vs parameter combinations becomes a plane with a triangular shape. The ARD values lead to different zones in the triangular plane, giving a patchy design where the darkest zones correspond to lower (and best) values. Even if the values remain close (between 41 and 64%), it is obvious that the optimal values are included in the 'valley' corresponding to the class 1 fraction around 35%. Four Vs combinations corresponding to fractions randomly selected in this 'valley' were used to select the Vs fractions for the step 2 (using two ViCAs). The combination giving the lowest ARD was taken (corresponding to the white circle for step 1 on Figure 6). One can note that the ARD found at this stage is slightly larger than the best ARD found in step 1 (around 41). Nevertheless, the choice to keep two different ViCAs depending on the wash-off and dilution period was made because it is presumed that it will be of great importance when integrating the model and simulating the PSVD evolution along the sewer and the WWTP during wet weather flow.

3.1.3. *Parameter set up*

The calibrated parameter values were used for the subsequent simulations. As explained earlier, Table 1 includes the thirteen parameters being calibrated plus the six fractions which are fixed by the Vs choice (in bold). The parameters in italics are fixed on the basis of a dedicated lab experiment. Their value is thus automatically set when the Vs class limits are set. The volume V_{Min} is close to what is expected from field observation, i.e. around 13 m^3 of stored water remaining in the PW after emptying.

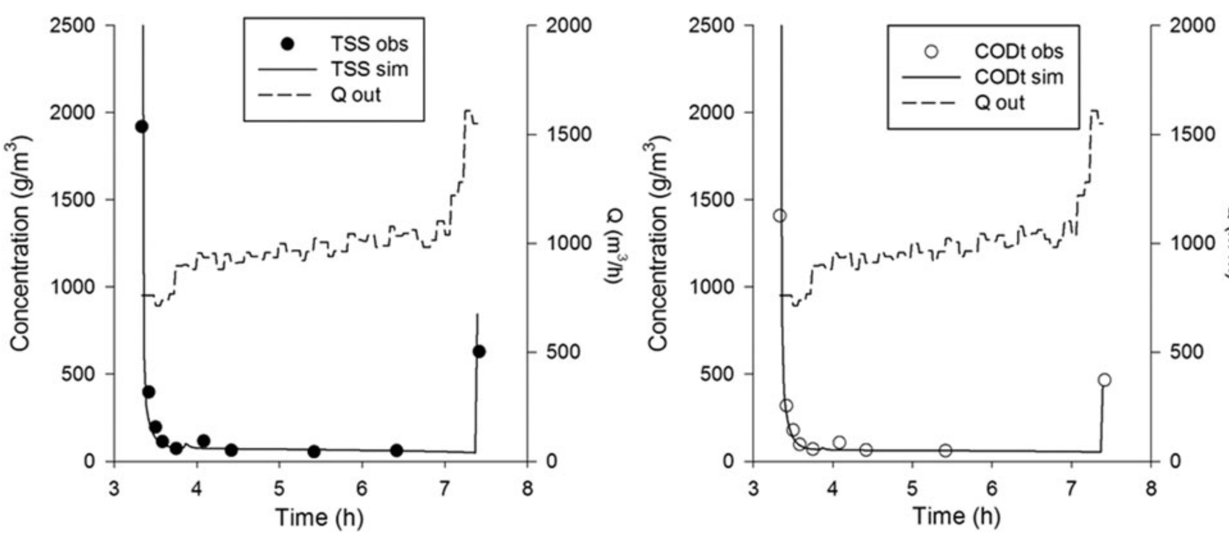

Figure 7. Calibration results for the July 27th 2009 event. a) On the left, the effluent TSS concentration, b) on the right, the effluent CODt concentration.

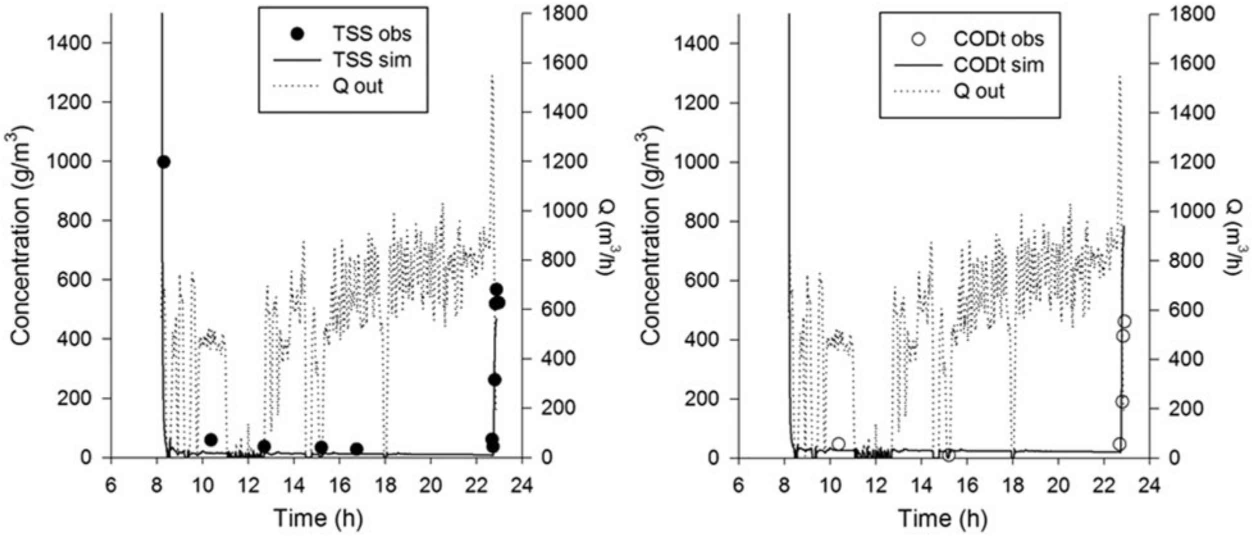

Figure 8. Calibration results for the September 27th 2009 event. a) On the left, the effluent TSS concentration, b) on the right, the effluent CODt concentration.

3.1.4. *Results of the calibrated model*

The calibration of the other parameters was carried out using two different events, of July 27th 2009 (Figure 7) and September 27th 2009 (Figure 8). The figures show the effluent concentrations, comparing the collected data against the simulated data. The two variables observed for this calibration are the TSS (on the left) and the CODt (on the right) concentrations. The pumped flow is represented by the dashed line.

Concerning the July 27th 2009 event, the emptying lasts around four hours without any interruption. It started about three hours and twenty minutes after water entered the tank. The outflow rate remained quite constant until the last fifteen minutes where it almost doubles. The first pollutant peak, resulting from the initial conditions, is well simulated. Indeed, that initial peak corresponds to the extraction of particles remaining in the PW from the previous event. To represent that initial mass, the model needs to set initial conditions. It is obvious that the Vs distribution is not equi-proportional for each class. Thus, a first warm-up simulation is run to set the particle distribution remaining in the PW as initial conditions for the real simulation (see Maruéjouls *et al.* 2012 for more details).

Emptying of the September 27th 2009 event lasts more than fourteen hours and starts around eight hours after

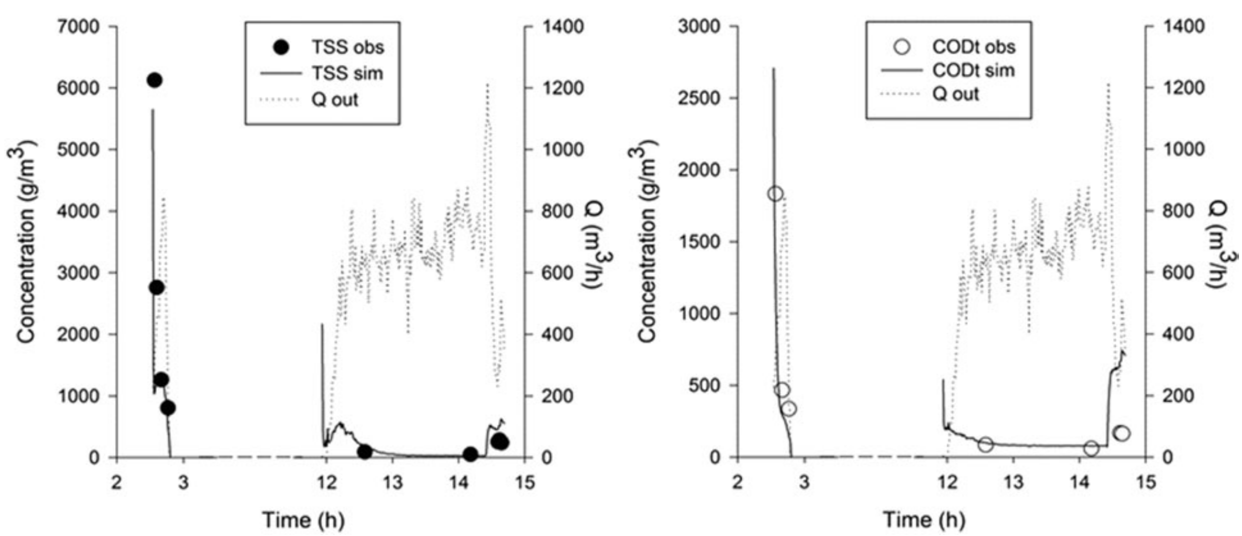

Figure 9. Validation results for the July 13th 2010 event. a) On the left, TSS effluent concentrations, b) on the right, CODt concentrations.

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filling had begun (Figure 8). That long emptying period is explained by many interruptions of the pumps due to several problems occurring in the field. The TSS concentration is slightly underestimated (for the lowest values, around 30 g/m^3 for the measurements and around 15 g/m^3 for the simulation). However, the CODt concentrations are quite well simulated, even at low concentrations.

One can observe the good fit of the model with the data collected for both of the events and for both TSS and CODt data. Nevertheless, it can be noticed that the CODt concentrations are better simulated during the middle periods of the emptying and during the final peaks.

3.2. Validation

The results of the validation using the parameters of Table 1 are presented in Figure 9. Emptying starts rather soon after the end of filling and lasts around nine hours. Actually, the total stored volume is emptied in two periods. The first pump activation lasts only for around 15 minutes and results in the '*initial*' peak (from 2.54 hours to 2.8 hours). A big part of the matter remaining in the PW from the previous event is then already evacuated. Nevertheless, the last fraction of the remaining matter plus the particles that settled during the ten hours of storage are extracted within the second emptying period, that starts around 12h00. This second concentration peak (at 12h00), which is actually a second '*initial*' phase, could not be validated by observations since none were collected. One can notice that for CODt, the final phase is overestimated by the model (around 800 g/m^3). It must be stated that the values observed in the field (TSS = 238 g/m^3 and CODt = 168 g/m^3) are lower than the usually observed ones that are around 500 g/m^3 (Maruéjouls *et al.* 2013).

4. Conclusion

The performance assessment of a new model describing pollutant behaviour in an off-line combined sewer retention tank has been carried out using full-scale field data. It is a 1-D phenomenological model requiring only a short simulation time. The pollutant evolution mechanisms are reproduced through three main processes: the sedimentation and resuspension of the particles, and hydrolysis of the biodegradable particulate COD. As far as the authors know, this is the first paper 1) proposing a method for the calibration of a retention tank model and 2) showing the results of its validation.

Retention tank emptying impacts both on the receiving body and the WWTP are an important issue of integrated wastewater management. This study illustrates the potential of such a model to properly describe the water quality in combined sewers and the influent quality of a WWTP. This model has been developed to allow its integration in a 'sewer – WWTP' system model. Different scenarios of emptying rules can now be tested to estimate the impact on the WWTP efficiency, i.e. scheduling the emptying of the different tanks in a sewer system in order to dilute the highest loads, or bypassing the less loaded volumes to minimize the shock loads at the WWTP.

This study provides a useful tool for integrated urban wastewater management, the performance of which has been assessed using full-scale field data. In the frame of a global approach, modelling establishes itself as essential for the understanding of wastewater engineering issues.

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