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Simulation of constructed wetlands treating combined sewer overflow using HYDRUS/CW2D☆,☆☆

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ABSTRACT

Constructed Wetland 2D (CW2D) is a biokinetic model describing microbial dynamics and transformation and degradation processes in subsurface flow constructed wetlands (CWs). The implementation of CW2D in HYDRUS (©PC Progress s.r.o.) was verified for application on CWs treating combined sewer overflow (CSO CWs). CSO CWs mitigate pollutant and hydraulic shock on receiving waters. Their loadings are stochastic in terms of periodicity, volume and quality. Their storage basin and outflow limitation causes cycles of saturated (intra-event) and unloaded (inter-event) states. The need for verification is due to this stochasticity. Key parameters to overcome the limitations identified by earlier studies were (1) biokinetic parameters, (2) fractionation of COD between readily and slowly biodegradable and inert forms and (3) adsorption of inert COD. With the new settings inoculation runs yielded stable biomass and domain conditions. These were successfully used as initial conditions for calibration and validation. Laboratory column experiments formed the basis of comparison, including single loads and a load series. The goodness of fit was quantified by an updated method. Good fit was reached to COD and NH_4-N. Fitting to NO_3-N was not a target; still, dynamics are discussed.

1. Introduction

1.1. Terminology and specificities of CSO CW

Combined sewer systems accommodate high flow rates of stormwater mixed with sewage during storm events. Therefore, these systems have to have integrated combined sewer overflow (CSO) mechanisms. On one hand these mechanisms prevent the overfilling of the sewer and surface flooding; on the other they limit flow rates to match the capacities of wastewater treatment plants. Peaks exceeding the hydraulic capacity of the plant are discharged as CSO (Meyer et al., 2013). If untreated, this flow is a significant pollution source (e.g. ammonium, organics) and hydraulic shock (e.g. streambed erosion and destruction of macroinvertebrate habitats) for receiving water bodies (Chocat et al., 1994).

Constructed wetlands (CWs) for CSO treatment are wide-spread or desired in several countries in Europe (Meyer et al., 2013). These systems differ in their loading characteristics from CWs treating sewage as CSOs have stochastic periodicity, volume and quality. CSO vertical flow CWs (here, CSO CWs) have a storage basin above the filter material. The high loading rates lead to saturated conditions of the media and generally to ponding above (intra-event state). Intra-event states last up to dozens of hours and are separated by periods up to dozens of days. In these, the filter media releases all gravitational water. The pores get filled with air and dry out to a various degree (inter-event state). The treatment processes can be attributed to either the intra-event or the inter-event environment based on their dominant occurrence. Filtration, adsorption and anaerobic degradation take place during the intra-event state. The porous media releases the water at a rate determined by an outflow throttle and aerobic processes, most importantly nitrification of the adsorbed ammonia dominate the inter-event state (Dittmer et al., 2005; Uhl and Dittmer, 2005;

☆ **Software**: HYDRUS 2D/3D 2.03.0350 and HYDRUS Wetland Module ©PC Progress s.r.o (hydrus@pc-progress.cz). Patch provided to (1) simulate outflow rate limitation and (2) to avoid hung occurring at *NH4N* depletion in the domain. For more details see http://www.pc-progress.com/en/Default.aspx?support.

☆☆ **Abbreviations**: model parameters, variables and components are written in *italic*.

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Meyer, 2011; Dittmer and Schmitt, 2011). Woźniak et al. (2007) reported however that aerobic processes may occur at both periods.

Constructed Wetland 2D (CW2D, Langergraber and Šimůnek, 2005) is a biokinetic model, implemented in the Wetland Module extension of the software HYDRUS (©PC Progress s.r.o). Referred to as HYDRUS/CW2D, it is designated to simulate CWs with continuous or frequent feeding patterns. Equations of water flow and reactive solute transport in HYDRUS are coupled with the aerobic and anoxic transformation and degradation processes and bacterial growth and decay of CW2D. The described pollutants are organic matter, nitrogen and phosphorus. Modelled bacterial groups are heterotrophs and two groups of nitrifiers (Langergraber and Šimůnek, 2011). For a more detailed process description, please refer to Langergraber and Šimůnek (2005, 2011).

The load pattern of CSO CWs is irregular leading to the stochastic alternation of intra- and inter-event phases. Still, HYDRUS/CW2D might be capable to simulate them because it has all sub-models of internal processes except the transport of particulates (filtration). The targeted pollutants in Germany and France, which are represented also in the tool, are COD and NH_4-N.

1.2. Previously identified limits of applying HYDRUS/CW2D on CSO CWs

One of our aims was to overcome previously identified limits, hence these limits are discussed here. The tool had been studied earlier to simulate CSO CWs. The simulations were based on laboratory column scale and pilot lysimeter scale experiments and had various successes (Henrichs et al., 2007, 2009; Meyer, 2011; Meyer et al., 2013). The previously applied calibration approach targeted stable biomass concentrations in CW2D. Loads and inter-event states were repeatedly simulated to reach biomass equilibrium. The outcome of such stabilization process can be used as initial conditions in order to see how the tool predicts the effluent concentrations after. This is a measure of the capability to simulate real series of CSO feedings using the HYDRUS/CW2D model package. The previously applied calibration approach included the following steps to reach stability:

1. Fitting flow and single solute transport using tracer test results.
2. Setting up sorption for *NH4N* and slowly biodegradable COD (*CS*).
3. Setting up COD fractionation.
4. Validation of the new parameters simulating other single events.
5. Validation via long-term simulations of consecutive events (reaching stability).

The calibration of the biokinetic parameters of CW2D was also listed in these works but it had been confused with setting up sorption, COD fractionation and manually setting bacteria initial conditions. Sorption is a submodel of the model package not related to CW2D; COD fractionation is about determining time-variable boundary concentrations manually and bacterium concentrations are variables of CW2D. The parameters of the biokinetic submodel were practically untouched and the limitations of HYDRUS/CW2D for simulating CSO CWs were drawn up like this.

Meyer (2011) was able to fit simulated and measured effluent concentrations of single loads. At first, initial bacterium concentrations were adjusted manually to match the vertical distribution of the measured DNA/RNA/ATP concentrations. Fitting this way was successful. Then, a similar biomass distribution was targeted via reaching biomass equilibrium. Fitting failed when using imported initial conditions from the stabilizing runs. Meyer (2011) (1) concluded the applicability of CW2D needs further simulation studies, (2) suggested an extension with particulate deposition and transport and (3) highlighted a gap in the knowledge about bacteria dynamics in the inter-event periods.

Henrichs et al. (2007, 2009) were successfully modelling ammonium dynamics and COD degradation when setting up adsorption for *CS*. A good fit was reached for single loads whilst long-term simulations failed for COD. Among the assumed causes were (a) COD fractionation of inflow between readily (*CR*) and slowly (*CS*) biodegradable and inert (*CI*) forms, (b) the concentration and distribution of heterotrophic biomass (*XH*) and (c) similarly to Meyer (2011), organic matter degradation and nitrification in inter-event periods.

CSO CWs differ in their loading and operation characteristic to normal CWs so the need of the calibration of the biokinetic parameters is anticipated. Issues (b) and (c) can theoretically be overcome adjusting biokinetic parameters which makes manual initial condition settings needless. Finding a balance between microbial growth and decay could put a cap on the limitless growth of *XH* as well and lead to realistic degradation rates in the inter-event periods. The calibration of a set of biokinetic parameters was targeted to obtain self-stabilized conditions, realistic biomass distribution and to provide a good match of simulated and measured effluent concentrations.

Our work targets to identify limits of the applicability of HYDRUS/CW2D on CSO CWs based on column experiment data and to bring closer full-scale applications. Using numerical models can give better insights to CSO CWs and understanding their limitations can promote model development itself (Meyer et al., 2015). Process-based models can be used to display detailed wetland functions but other necessities might need different approaches. In the case of CSO CWs, displaying long-term purification efficiencies was found highly important in a phenomenological model for design-support (Meyer and Dittmer, 2015).

2. Materials and methods

2.1. Experimental set-up

The laboratory columns and experimental data on loads (Woźniak, 2007, Woźniak et al., 2007) were selected from a long-term project series ('BOFI') carried out at the Institute of Urban Water Management, University of Kaiserslautern, Germany. The columns (Fig. 1) had outflow limitation and rapid loading pulses which resulted ponding above the sand filter media. Loads were wastewater diluted to concentrations which is typical for CSOs (Dittmer et al., 2005).

CW2D was used in the version 2.03 of HYDRUS with a patch enabling to simulate outflow limitation by setting up an upper threshold on the outflow rate. Another patch prevented the calculations to halt when ammonium-nitrogen in the model (*NH4N*) was depleted. To be able to compare the previous simulation study of Meyer (2011) to the present one an identical domain was created. It consisted of 3×105 (horizontal $\times$ vertical) finite elements as represented on Fig. 1. The storage volume above the filter media was substituted by a material with no residual water content ($Q_r = 0$); hundred per cent porosity ($Q_s = 1$) and a high hydraulic conductivity at saturation ($K_s = 104$ m/h) ('air layer'). The outflow was throttled to 0.01 or 0.03 L/s/m^2.

2.2. Used calibration and validation approach

The simulation study had three main work phases: (1) reproduction of the simulations of Dittmer et al. (2005) and Meyer (2011) (see also Section 1.2) with identical parameters to verify new software version and patches, (2) calibration of parameters to achieve biomass equilibrium and a good fit of a following single load, and (3) validation of the new biokinetic parameter set using other single loads and a load series of five loads. The targets of fitting were

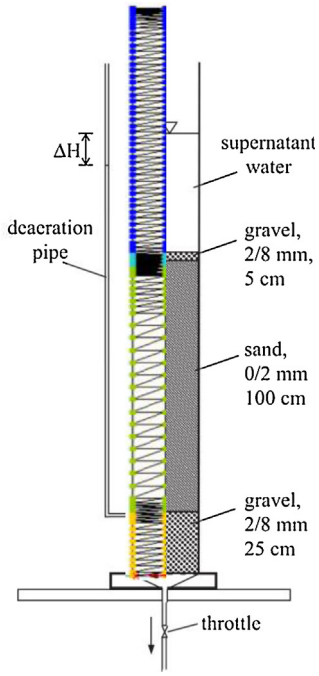

Fig. 1. Section draft of the physical columns (based on Meyer, 2011). $D = 19$ cm. The left side to the symmetry axis is swapped to the left half of the finite element mesh used in the simulations.

measured COD and NH_4-N concentration series in the effluent. The goodness of fit was evaluated also to measured NO_3-N concentration series.

Water flow, solute transport (based on tracer curve) and sorption parameters of *NH4N* and *CS* were accurate and thus taken unchanged from Meyer (2011). These are essential to set properly when modelling any CWs. Earlier limitations were related to heterotrophs (*XH*), total COD (*CR* + *CS* + *CI*) and possibly the lack of filtration processes. As such, the targets of the calibration were identified to be (1) to eliminate exponential biomass growth of *XH*, (2) to overwind the lack of filtration of the particulates, (3) to match the distribution of the simulated biomass to measured vertical DNA, RNA and ATP concentration profile, (4) to flatten an early outwash peak (flush) of COD in the simulated effluent which is absent in the reality and (5) to achieve a good fit to single loads and a series of loads without setting initial bacterium concentrations manually.

The possibly relevant parameters based on the mathematical formulations of the biokinetic model CW2D (Langergraber and Šimůnek, 2005, 2011) were anticipated to be:

a) μH: maximum aerobic growth rate of *XH* on readily biodegradable COD (*CR*);
b) *bH*: rate constant of lysis for *XH*;
c) *rate_O2*: re-aeration rate;
d) Y_x: Yield coefficient for *XH* (heterotrophs), *XANs* (*Nitrosomonas*) and *XANb* (*Nitrobacter*);
e) *CR:CS:CI*: fractionation of the COD load to readily and slowly biodegradable and inert.

The simulation domain was loaded with 0.5 m^3/m^2 every fourth day to reach a stable biomass. Biokinetic parameters were adjusted manually such that the final biomass matches the vertical distribution of the measured DNA, RNA and ATP concentrations shown by Meyer (2011) and Woźniak (2007). The stability meant the elimination of limitless growth (Samsó and Garcia, 2013) as well. The cyclic loads targeted to reach a stable biomass starting from a bacterium concentration of 1 μg COD per g media for *XH* (heterotrophs), *XANs* (*Nitrosomonas*) and *XANb* (*Nitrobacter*). The final, stabilized condition of the last cycle (balance of growth and decay in the cycle) was used as initial condition for the calibration and validation runs.

Table 1
Characteristics of the single events (1–4) and the event series (5) used for validation.

#	Index of the column event		Time from the previous load [days]	Loading height [mm]	Flow limitation [L/s/m²]
1	S1	ES08	(4)	750	0.03
2	S1	ES40	(4)	2500	0.01
3	S3	ES35	(4)	1500	0.03
4	S3	ES36	(4)	1000	0.03
		ES32	(4)	1500	
		ES33	7	500	
5	S1	ES34	2	500	0.01
		ES35	5	2200	
		ES36	7	1000	

The same high load was used for calibration as in Meyer (2011) (code "S1 ES35" – first column, 35th load in the physical experiments). Bacterium distribution and activity were targeted to match measured values. In reality, bacterial dynamics are not exactly known during loadings and inter-event periods. For these reasons, the composition of COD produced by biomass lysis was set to 99.999% *CI* which enables to see decay products separately when refining parameters or interpreting results. It was learnt, a much lower simulated biomass has to be targeted to flatten the peak of *CI* built up during the inter-event lysis. To achieve it, a simple sensitivity analysis (SA) had been carried out on the yield coefficient of heterotrophs (*YHet*) and the COD fractionation (*CR:CS:CI*) which were seen as key parameters. The goal of the SA was to increase the understanding of the effect of these two input parameters on the output concentrations. The analysis consisted of running simulations with three values of both parameters. Then, refinement of other parameters and validation could follow.

Table 1 summarizes the characteristics of the real loads randomly selected for validation. Many of these were extreme in terms of filtered volumes. The validation aimed to reproduce effluent concentrations from single loads (#1–4) and a complete series of loadings (#5), all starting from the self-stabilized initial concentrations. Simulations of stand-alone loads involved setups with two different outflow limitations. The series included the load S1 ES35. This load is for which the calibration was done, but this time its initial conditions were shaped by the preceding loadings instead of stabilizing runs.

2.3. Numerical evaluation of goodness of fit

The coefficient of efficiency (E_j) was calculated without exponential ($j = 1$) which form is more sensible to fitting inaccuracies (Ahnert et al., 2007). Composite samples represent various time intervals; this was counterbalanced by adding time-weighing to Eq. (1) which is the classical equation:

$$E_j = 1 - \frac{\sum_{i=1}^{n} |M_i t_i - E_i t_i|^j}{\sum_{i=1}^{n} |M_i t_i - \bar{M} t_i|^j} \quad (1)$$

where M_i is the measured value, E_i is the simulated value, $\bar{M}$ is the time-weighted average of the measured values, and t_i is the time represented by composite *i*. E_i t_i is calculated from several values falling in the time span of composite *i* by taking their numerical integral by time.

Ahnert et al. (2007) give no range to evaluate goodness of fit based exclusively on the values of E_j. They suggest to couple it with other numerical methods and it is important to have a visual depiction as well. The value of E_j is below zero when the arithmetic mean

Table 2
Settings of the calibration process targeting to remove the initial COD peak and to reach an overall good fit.

#	Base	Parameter	Symbol	Adjustment [%] or [N/A]	New value
SA1a	Stable biomass	Yield coefficient for *XH*	*YHet*	−25	0.39
SA1b	Stable biomass	Yield coefficient for *XH*	*YHet*	−40	0.31
SA1c	Stable biomass	Yield coefficient for *XH*	*YHet*	−50	0.26
SA2a	SA1c	*CR:CS:CI* ratio (inflow)	–	Original ratio	60:20:20
SA2b	SA1c	*CR:CS:CI* ratio (inflow)	–		40:40:20
SA2c	SA1c	*CR:CS:CI* ratio (inflow)	–		30:60:10
SA1d	SA2c	Yield coeff. for *XH*	*YHet*	−88	0.065
		Yield coeff. for *XANs*	*YANs*	−75	0.060
		Yield coeff. for *XANb*	*YANb*	−75	0.060

of the measurements is a better predictor than the model (Ahnert et al., 2007). This normally indicates a bad fit but it was noticed this happens also if the measured values are very low or the concentrations are closely constant. The interpretation of E_j was aided by calculating the mean time-weighed deviation as shown on Eq. (2).

$$\overline{DEV} = \frac{\sum_{i=1}^{n} |M_i t_i - E_i t_i|}{t} \quad (2)$$

where t is the duration of the intra-event period on which the analysis is done. The deviation was expressed as the percentage of the time-weighted mean of the measured values as well. $\overline{DEV}$ [mg/L] and $\overline{DEV}$ [%] are easy to interpret and in the case when E_j is around or below zero they show if the fit is really weak or E_j fails because near constant or very low measured values. The goodness of fit was considered weak if E_j indicated weak/mediocre results with a value below 0.1 and $\overline{DEV}$ [mg/L or %] seemed important.

3. Results and discussion

3.1. Test runs with identical settings to previous investigations

XANs and *XANb* (*Nitrosomonas* and *Nitrobacter*, respectively) concentrations were reaching stability with standard biokinetic parameters. Indeed, Henrichs et al. (2009) fitted *NH4N* already and concluded that further work should target long term simulations of stochastic intra- and inter-event patterns. Reproducing COD concentrations had been proven to be more difficult. With these settings, just as in Meyer (2011) and Henrichs et al. (2007), the equilibrium of *XH* could not be reached and the initial flush of COD was also experienced.

3.2. New parameter set for CSO CWs

A new parameter set was developed which led to a realistic biomass distribution and activity along the vertical profile. The values of heterotrophic yield coefficient (*YHet*) and *CR:CS:CI* ratios used during the calibration process are summarized in Table 2. The early flush of COD was addressed by decreasing *YHet* (sensitivity analysis runs SA1a-SA1c). This change had boosted substrate digestion by a unit of bacteria. It also helped to reproduce the vertical pattern of biomass distribution: more nutrients were used at the top whilst the wastewater was flowing through. This created starvation deeper. The setting slightly decreased the predicted treatment performance as a side effect. The sensitivity analysis on COD fractionation made possible to counterbalance this (sensitivity analysis runs SA2a-SA2c). The new fractionation allowed to decrease *YHet* further and thus to obtain an even better fit. This time autotroph yield coefficients (Y_{ANs} and Y_{ANb}) were decreased proportionally to maintain a realistic ratio of mass (Langergraber, 2001) between heterotrophs and autotrophs (SA1d).

The setup SA1d gave an acceptable fit with a shrunk initial COD peak. The ratio of *CI* generated by lysis was set utmost high; still, this COD was not only *CI* but added up from *CI* and *CR*. To remove the residual peak, a low linear adsorption capacity was set for *CI*. *CI* can be interpreted as particulates which are less mobile than dissolved decay products represented by the initial peak of *CR*. Fournel (2012) observed initial COD peaks consisting of both particulate and dissolved forms in pilots mentioning hydraulic shortcuts as potential cause. Setting non-zero adsorption capacity for the inert COD fraction (*CI*) is necessary when there is no particulate breakthrough, otherwise, like in the case of Fournel (2012), could be left zero.

In total, eleven biokinetic parameters were adjusted plus adsorption was set for *CI*. This (1) smoothened the residual peak of COD, (2) eliminated the exponential growth with a realistically distributed biomass and (3) led to a good fit of simulated and measured values. The changes are summarized in Table 3, compared to the original parameters (unchanged biokinetic parameters of program version 1.xx) used by Meyer (2011). The description of the effect and/or a short rationalization is given for each adjustment.

3.3. Biomass development

The biomass had reached stability within 40 cycles of repeated loads (160 days) which matches the length of the inoculation period of the real columns (Woźniak, 2007). The final ratio of heterotrophs (*XH*) to autotrophs (*XANs* + *XANb*) at −1.5 cm was realistic with 8:1 (Langergraber, 2001). The distribution of the biomass followed the vertical distribution of the measured DNA, RNA and ATP concentrations during the last inter-event period (Fig. 2). Nutrient availability along the vertical profile is represented well by the distribution also in the simulations. The weight of the simulated biomass is expressed in μg COD per g filter media and direct comparison is not possible with measured DNA/RNA/ATP values expressed in μg per g.

3.4. Calibrated results for S1 ES35

The calibrated HYDRUS/CW2D parameters led to a good fit between the simulated and the measured effluent concentrations (Fig. 3). The initial conditions were imported from stabilization runs. Adsorbed *NH4N* concentrations had to be manually adjusted if they were near zero (after full nitrification) to 0.4 μg/g in order to avoid numerical problems. Simulated values match the measured effluent COD and NH_4-N. Note the low peak which is the residue of the initial COD (*CR* + *CS* + *CI*) flush between 3 and 6 h event time (at 15 mg/L; original peak: 85 mg/L).

3.5. Validation with single loads

The validation of the new parameter set included the simulation of other loadings with the same setup. The effect of different throttle values is compared on Fig. 4. The effluent COD matches the measured values with a good accuracy in the case of the 0.01 L/s/m^2 flow limitation and with an excellent accuracy in the case of the 0.03 L/s/m^2.

Table 3
Parameters of HYDRUS/CW2D adjusted for simulation of CSO CWs compared to the original values in Meyer (2011) and the effect and rationalization of the adjustments.

Parameter	Original value	New value	Effect and rationalization
Hydrolysis rate constant, K_h [1/d]	0.05	0.2	Prohibits the separation of two bacterium-rich layers near the top of the column feeding on direct *CR* input and hydrolysis product *CR*
Maximum aerobic growth rate of *XH* on *CR*, μ_H [1/d]	0.1	0.042	Balances intra-event growth and inter-event decay to avoid unlimited growth, affects the maximum *XH* concentrations
Maximum aerobic growth rate of ammonia oxidizing bacteria, μ_{ANs} [1/d]	0.015	0.025	Balances the growth with the inter-event decay to avoid the diminishing of *XANs*
Half-saturation coefficient for *SO* of ammonia oxidizing bacteria, $K_{ANs,O2}$ [mg/L]	1	0.066	Enables *XANs* to grow during and after the loadings, low value was calibrated also by Pálfy and Langergraber (2014)
Maximum aerobic growth rate of nitrite oxidizing bacteria, μ_{ANs} [1/d]	0.017	0.04	Balances the growth with the inter-event decay to avoid the diminishing of *XANb*
Half-saturation coefficient for *SO* of nitrite oxidizing bacteria, $K_{ANs,O2}$ [mg/L]	0.1	0.066	Enables *XANb* to grow during and after the loadings.
Fraction of CI generated in biomass lysis, $f_{BM,CI}$ [–]	0.02	0.99999	Enables to tackle the initial flush of COD in two fractions separately which are *CI* and *CR* instead of *CR* only
Fraction of *CR* generated in biomass lysis, $f_{BM,CR}$ [–]	0.1	10^{-6}	*CR* + *CI* must be smaller than 1
Yield coefficient for *XH*, Y_{Het} [–]	0.65	0.065	Decreases biomass without compromising treatment efficiency and flattens the initial peak of COD; leads to more biomass closer to the inlet
Yield coefficient for *XANs*, Y_{ANs} [–]	0.24	0.06	Decreases biomass without compromising treatment efficiency, flattens the initial peak of COD, helps to keep the ratio of heterotrophs and autotrophs realistic
Yield coefficient for *XANb*, Y_{ANb} [–]	0.24	0.06	
Adsorption capacity of sand for *CI*	n/a		Flattens the initial flush of COD with unperceivable
Kd [cm³/g]		0.2	effect on any of the estimated treatment performances
Beta [–]		1	during the whole event
Alpha [1/h]		1	

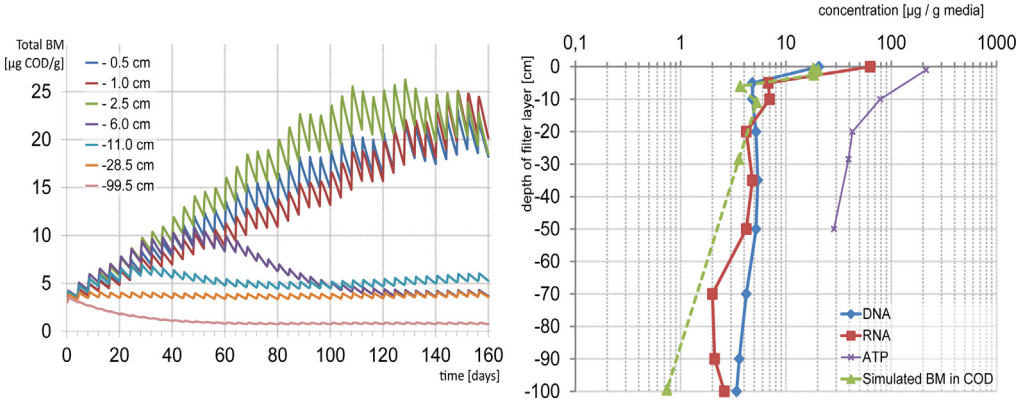

Fig. 2. Biomass (BM) development and vertical distribution at equilibrium. Simulated concentrations during 160 days of inoculation (left) and comparison of the final distribution at day 160 with DNA, RNA and ATP measurements (Woźniak, 2007) along the vertical profile of the filter (right). (For the colours on the left chart, the reader is referred to the web version of the article.)

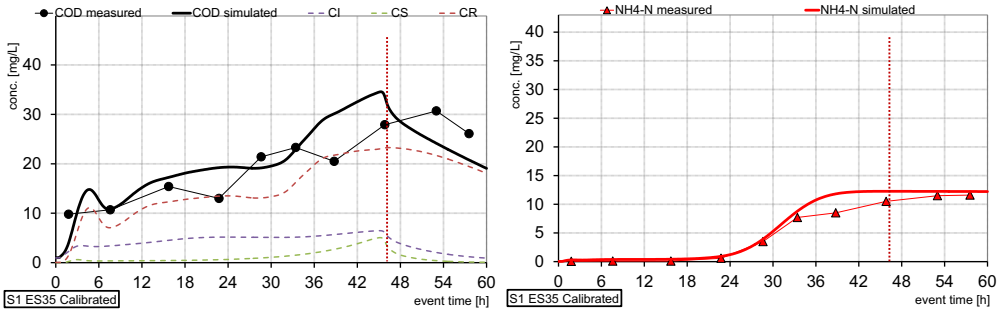

Fig. 3. Calibration results on COD and NH_4-N. The red dotted line marks the outflow rate getting lower than the flow limitation. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

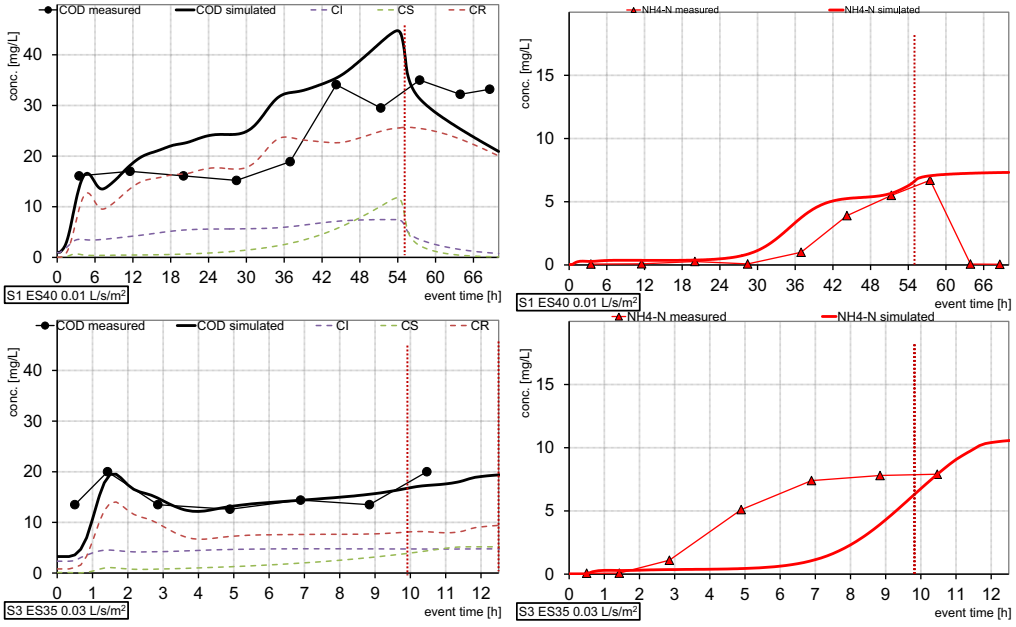

Fig. 4. Validation results from domains with different flow limitaions. Top: 0.01 L/s/m^2, bottom: 0.03 L/s/m^2, left: COD and COD fractions, right: NH_4-N.

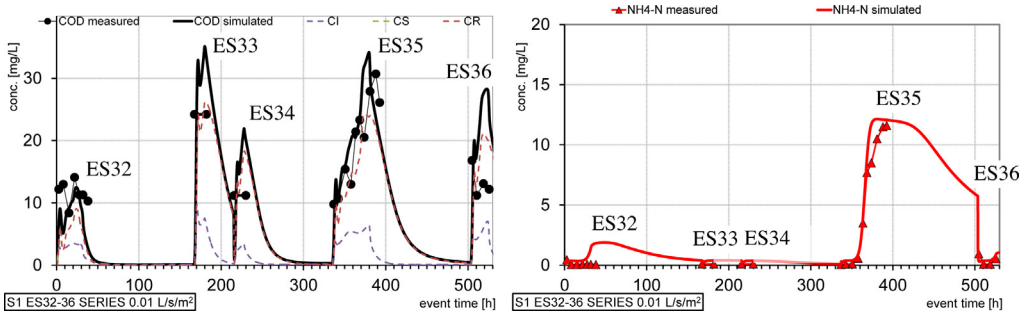

Fig. 5. Model validation with a series of five consecutive loadings, ES32-36. Simulation is continuous but measurements were made during the intra-event periods exclusively.

The ammonium nitrogen concentrations show an excellent fit at 0.01 L/s/m^2 whilst a slight mismatch in both the beginning and the maximum values of the breakthrough at 0.03 L/s/m^2. Woźniak (2007) concluded that 0.03 L/s/m^2 is already a critical operational condition where preferential flows start to be significant. In fact, preferential flows and hydraulic shortcuts mean less contact surface and time for adsorption leading to earlier breakthrough. They also mean more passive pores which flattens the initial NO_3-N peak because the washout needs more time. The lower fit can be explained by critical hydraulic operation because preferential flow is not implemented in HYDRUS/CW2D. Furthermore, tripling the flow rate means a shorter time on the same bar increasing our visual sensitivity to errors.

Woźniak et al. (2007) reported an oxygen reservoir in the filter media which depletes with time and effects the breakthrough of NH_4-N. This reservoir is correlated to the shape and size of the grains and assumedly to the outflow limitation as well. Based on possible critical hydraulic operation and the existence of the oxygen reservoir it is recommendable to re-calibrate *NH4N* adsorption for different materials and flow limitations.

3.6. Validation with load series

The results are shown on Fig. 5 where five loadings (see Table 1) are each represented by a peak. The simulated values are concentrations at an outlet node so there is continuous prognosis, still, attention should be paid only where measured values are given (full-toned sections of the series). The first simulated load (ES32) is equivalent to a single load as it follows directly a stabilization run. The second and the third loads (ES33 and ES34) were sampled only as full event composites. Most important are the predictions for the fourth and fifth events (ES35 and ES36). The initial conditions of these bear the effect of the previous loads. The predicted COD and *NH4N* concentrations are very well fitted in ES35. ES36

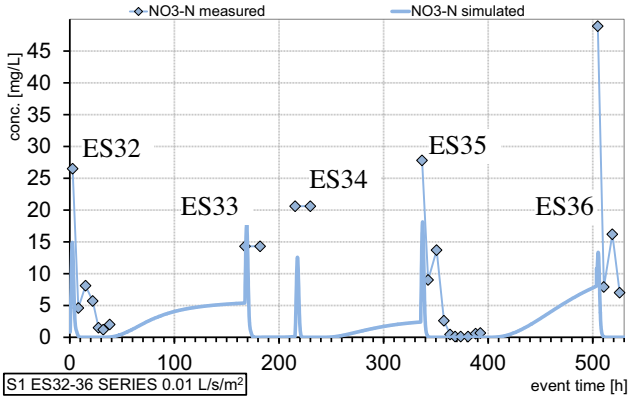

Fig. 6. Comparison of measured and simulated flush of NO_3-N of five consecutive loadings, ES32-36.

Table 4
Numerical evaluation of the goodness of fit. **Green: good fit,** ochre: moderate fit, *pink: weak fit*. The outlines mark the crucial value on which the categorization was based.

Index of the		E1 -			DEV [mg/L]			DEV % of t.w.mean		
column	event	COD	NH_4-N	NO_3-N	COD	NH_4-N	NO_3-N	COD	NH_4-N	NO_3-N
S1	**ES35**	**0.49**	**0.73**	0.27	**3.15**	**1.22**	4.62	**15%**	**23%**	85%
S1	**ES08**	**0.20**	**-11.30**	0.20	**2.79**	**0.24**	4.98	**16%**	**369%**	68%
S1	**ES40**	**0.31**	**0.21**	0.17	**6.85**	**2.01**	4.30	**25%**	**102%**	97%
S3	ES35	**0.22**	0.08	*-6.85*	**1.93**	2.67	*4.54*	**13%**	56%	*82%*
S3	ES36	**-2.73**	**0.22**	*-0.10*	**3.65**	**1.40**	*13.90*	**21%**	**64%**	*90%*
S1	**ES32**	**-1.35**	**-3.80**	-0.13	**3.52**	**0.50**	6.61	**30%**	**391%**	84%
	ES33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	ES34	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	ES35	**0.39**	**0.81**	0.33	**5.15**	**1.10**	5.53	**21%**	**17%**	84%
	ES36	*-6.68*	**0.14**	*-0.39*	*10.76*	**0.26**	*15.69*	*83%*	**74%**	*90%*

provided weaker results for COD: outflow concentrations were overestimated. *NH4N* fits very well.

The simulations put the intensive nitrification at the first part of the inter-event periods. *NO3N* concentrations fit weakly (Fig. 6), even though they reflect the experienced flush-out dynamics. The peaks are lower than the measured and their duration is shorter. This means a lower mass of nitrate-nitrogen is leaving the system in the model than in the reality (e.g. ES36: 42 mg against 476 mg, respectively).

3.7. *Goodness of fit*

Table 4 contains the numerical evaluation of the goodness of fit. The fit for COD is good except the case of S1 ES36 in the series where COD concentrations were overestimated. *NH4N* fits well to the measured values and the best estimation is given for this parameter even if the breakthrough was predicted late in the case of S3 ES35. The weakest predictions are given for NO_3-N where the trend follows the measured but the initial peak is underestimated in both magnitude and duration.

4. Conclusions and outlook

It was possible to reach a quasi-stable biomass distribution in CSO CW domains by self-regulating inoculation runs. Reaching stability needed the adjustment of biokinetic parameters. The inoculation runs were repeated simulations of the same intra- and inter-event periods. A realistic vertical distribution comparable to measured DNA, RNA and ATP concentration did not reside in equilibrium. This needed further calibration. The abundance of biomass was underestimated: the measured RNA had a higher density in μg/g than the simulated total biomass in μg COD/g. The parameter set leads to underestimated bacterial concentrations but realistic vertical distribution and removal activity.

HYDRUS/CW2D was capable to simulate CSO column performance for COD and NH4-N removal after reaching biomass stability. The previously experienced unlimited growth of biomass and the overestimated initial peak of COD were overcome simultaneously by (1) adjusting biokinetic parameters, (2) calibrating COD fractionation (*CR:CS:CI*) and (3) setting a low adsorption capacity for inert organics (*CI*). The simulated COD and *NH4N* concentrations fit well or moderately the measured ones.

Fitting *NO3N* was not targeted by this study and needs further research. Still, the load series ES32-36 represented a closed material balance and thus conclusions could be made. The nitrate flush was underestimated in terms of concentrations and duration. Denitrification was uncalibrated and heterotrophs (*XH*) transformed about 2/3 of *NO3N* and produced *N2*. Calibrating denitrification would be essential to have a better fit as there was no denitrification observed in the reality. Furthermore, Fournel (2012) and Meyer (2011) concluded that organic nitrogen degradation is a main driving factor behind nitrate releases. As *CS* is degraded in the inter-event periods, increasing the parameter representing its nitrogen content ($i_{N,CS}$) should result more *NO3N* is flushed out.

The filtration of particulates is a main treatment process of CSO CWs inexistent in HYDRUS/CW2D. This deficiency was neutralized by new values of biokinetic parameters and the adsorption processes set for COD (*CR* + *CS* + *CI*). Attention should be paid to the fact that pre-settled water was loaded on the columns. Other setups, e.g. French CSO CWs receive unsettled water and higher concentration of TSS. The new parameter set waits to be verified for these systems and further adjustments might be necessary.

The hydrolysis rate seemed to be independent from nutrient availability and water content in the model. This enabled complete *CS* hydrolysis even in the long inter-event periods. Hydrolysis would go on even if the domain dries out and this is unrealistic. Hydrolysis should be dependent on the water content, e.g. by adding a half-saturation coefficient. Nutrient dependency of hydrolysis is to be considered as well to see if the enzyme production of heterotrophs (*XH*) should be made dependent from the availability of nitrogen components. These two extensions might allow to use the original fractions of COD generated at bacterial lysis instead of making *CI* dominant. If the initial peak from the washout had been *CS* instead of *CR* it would have been flattened due to the *CS* adsorption capacity set.

Validation on full-scale systems should follow. Using HYDRUS/CW2D on full scale should help to improve CSO CWs design and operation scheme. For design purpose, the parameters might be fine-tuned again based on the national standards. For example, the French system has a courser media, permanently saturated water layer at its bottom and receives unsettled CSO and this is plenty of differences compared to the German CSO CWs.

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