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Model Study of Short-Term Dynamics of Secondary Treatment Reed Beds at Saxby (Leicestershire, UK)

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Relatively simple black-box models, such as the well-known k-C* model, are commonly applied to design horizontal sub-surface flow constructed treatment wetlands. Important shortcomings of this model are the oversimplification of reality on the one hand, and the inability to predict short-term effluent dynamics on the other. A possible solution for these drawbacks could be the application of dynamic compartmental models. This article reports on the calibration requirements and the simulation results of such a dynamic model. A quantitative sensitivity analysis was used to identify the most sensitive parameters after which model predictions were optimized by adjusting those parameter values. Model fits were acceptable but missed some of the short-term dynamics observed in reality. At this point, it might therefore still be unwise to use the model as a design tool. Further model adjustments and calibration efforts are needed to enhance its reliability.

Key Words: Constructed treatment wetlands; Wastewater; Dynamic compartmental models; Calibration.

INTRODUCTION

The increasing application of constructed wetlands for wastewater treatment coupled to increasingly strict water quality standards is an incentive for the development of better design tools. Originally working with rules of thumb and

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simple regression equations, most researchers and designers evolved towards the use of the well-known first-order k-C* model.[1] This black-box model however is based on only two parameters, the first-order decay rate k, and the background concentration C*, which is an obvious oversimplification of the complex wetland processes. Kadlec also proved that the so-called rate constant k was not constant at all, but depends on factors such as loading rate, inlet concentrations, etc. The addition of an extra parameter did not improve the model output.[2] A design case study by Rousseau et al.[3] clearly demonstrated that the predicted required surface areas by applying these rather simple design models are extremely variable. This variability did not only occur between the different model types, but due to parameter uncertainty also within the same model category.

During the last couple of years, several dynamic, compartmental models of horizontal subsurface flow or so-called root-zone constructed treatment wetlands (HSCTW) have been presented in the literature.[4,5] These models explicitly take into account the different processes occurring in constructed treatment wetlands. Simulation results of these models seemed quite promising. They however have one major drawback: several dozens of parameters need to be estimated. A sensitivity analysis can reveal those insensitive parameters that do not require a very accurate estimation. Parameters, on the other hand, having a major influence on the model output have to be determined precisely.[6] Since little has been published about the values of most of these parameters, calibration must be based on input–output data. Up to now, dynamic constructed treatment wetland models are therefore quite useless as design tools.

This article reports on a research project that was aimed at extending and calibrating an existing dynamic model of a HSCTW and at checking whether or not the model output would be good enough to use the model as a design tool. First, the survey results of the test site are briefly summarized and important processes are indicated. Then the model structure is outlined, the calibration procedure is described and simulation results are given. Finally, during the discussion, some model flaws and calibration difficulties are identified and the applicability of the model for design purposes is assessed.

MATERIALS AND METHODS

In August 2002, a detailed data set was collected at a two-stage reed bed of Severn Trent Water Ltd. at Saxby (Leicestershire, UK), a constructed treatment wetland designed for 47 population equivalents (PE) and in service since 1998. The system consists of two horizontal sub-surface flow beds connected in series, preceded by a conventional septic tank for primary treatment. Each bed has a surface area of 117 m^2 and an average depth of 0.6 m (Fig. 1). Prewashed 5–10 mm gravel is used as filter medium. Wastewater is distributed over the entire

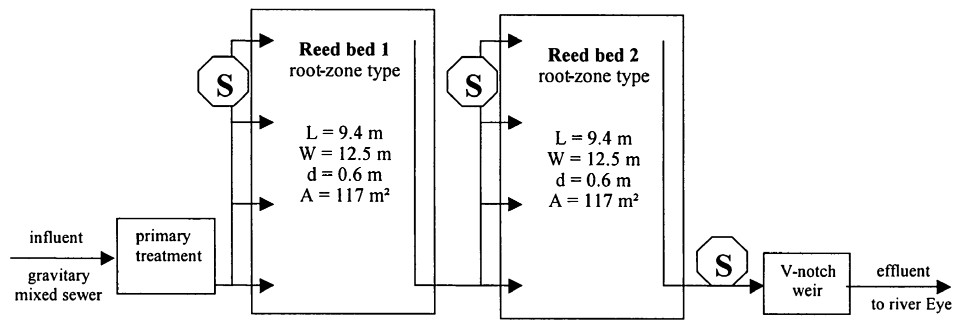

Figure 1: Schematic representation of the constructed treatment wetland in Saxby. S indicates location of samplers.

width of the reed beds via an aboveground trough with equidistant V-shaped openings.

A two-week survey was carried out during which eight-hour composite samples were collected of the presettled influent, the effluent of the first bed and the effluent of the second bed (Fig. 1). Noncooled automatic samplers were used. They were programmed to take one sample of 125 ml every hour and to combine 8 samples in one bottle. Composite samples were preferred because they facilitate the application of mass balances and they correspond better with the step inputs that are commonly used in simulation software. Samples were then taken to the lab on Monday, Wednesday, and Friday, and were thus a maximum of 2.5 days in nonrefrigerated conditions. All samples were sent to Severn Trent Laboratories and analyzed for total and filtered biochemical oxygen demand (BOD_t and BOD_f), total and filtered organic carbon (TOC_t and TOC_f), suspended solids (SS), ammonium (NH_4-N), total oxidized nitrogen (TON), total nitrogen (TN) and orthophosphates (ortho-P). Occasionally, total chemical oxygen demand (COD_t) analyses were carried out.

Effluent flow rates of the second reed bed were measured every 15 minutes by means of a V notch weir with an angle of 28.1° and an ISCO Model 4230 Bubbler Flow meter (Fig. 1), the latter device being more suitable to measure low flow rates. Simultaneously, meteorological data were collected since these have a major impact on the water balance. Precipitation was measured via an ISCO Model 674 tipping bucket rain gauge attached to the flow meter. Other meteorological data, i.e. air temperature and day length, were gathered via meteorological sites on the Internet.

SURVEY RESULTS

The daily average air temperature during the survey varied between 12°C and 30°C. Some severe rainstorms occurred on August 8 and 9, which forced the

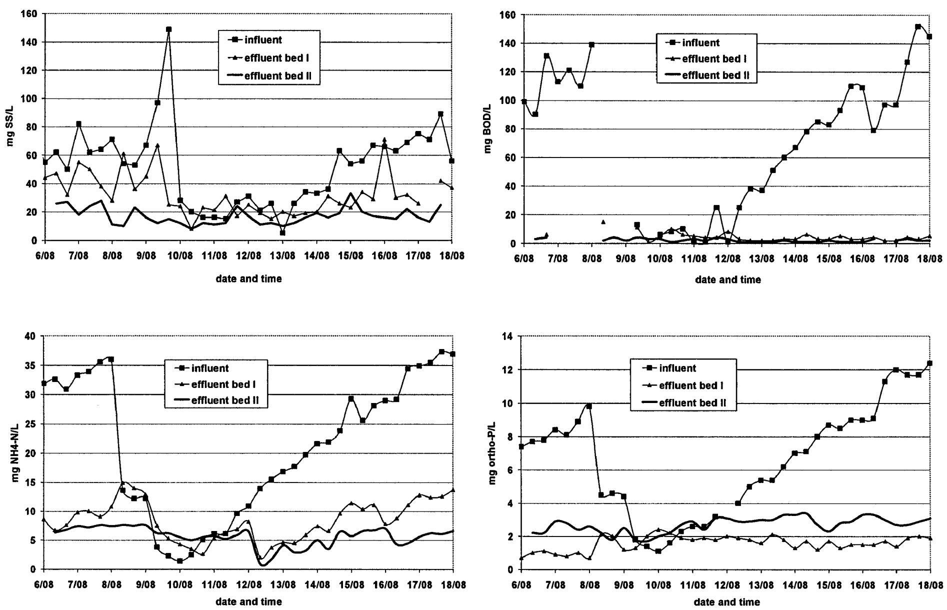

Figure 2: Concentration time series of SS, BOD, NH_4-N and ortho-P, measured at the constructed treatment wetlands in Saxby from August 6 to 18, 2002. Data from presettled influent, effluent of the first reed bed, and effluent of the second reed bed.

influent flow rate from a base flow of less than 0.1 l s^{-1} to a peak flow of about 15 l s^{-1} since no combined sewer overflow or bypass is provided. Corresponding hydraulic loading rates varied from as low as 5 cm day^{-1} up to about 100 cm day^{-1} during storm events. This caused temporary flooding of the beds. The treatment works nevertheless consistently produced a high quality effluent with BOD and SS concentrations lower than 10 mg l^{-1} and 30 mg l^{-1}, respectively. Ammonium-nitrogen and ortho-P concentrations also were relatively unaffected by the fluctuating flow rates and varied between 0.9 and 7.6 mg N l^{-1} and 1.4 and 3.7 mg P l^{-1}, respectively (Fig. 2). Remarkably, phosphorus concentrations in the effluent of the second bed are consistently higher than those of the first bed, indicating a net phosphorus production in the second bed. All in all, this constructed treatment wetland seems to have a considerable hydraulic buffering capacity.

Average BOD, NH_4-N, TON ($=NO_3 + NO_2$), TN, and ortho-P removal efficiencies (Table 1) can be called excellent with reference to reported literature values. SS removal on the other hand seems to be only average. When looking in terms of mass removal, this constructed treatment wetland is capable of removing 67.9 kg SS ha^{-1} d^{-1}, 18.2 kg BOD_t ha^{-1} d^{-1}, and 3.6 kg TN ha^{-1} d^{-1}. These figures clearly indicate that the beds have enough oxygenation capacity but on the other hand also provide enough anoxic regions where denitrification takes place.

Table 1: Average removal efficiencies of the constructed treatment wetlands in Saxby, based on average concentrations (in %).

	Inlet ($mg\ L^{-1}$)	**Outlet Bed I ($mg\ L^{-1}$)**	**Outlet Bed II ($mg\ L^{-1}$)**	**Removal (%)**	**Mass removal ($g\ ha^{-1}\ day^{-1}$)**
TON	0.9 ± 1.5	2.5 ± 2.7	1.1 ± 1.4	−25.3	1.1
SS	52.7 ± 28.0	32.4 ± 14.8	16.6 ± 6.7	68.5	67.9
BOD_t	73.7 ± 47.2	4.6 ± 3.1	2.1 ± 1.0	97.1	18.2
BOD_f	52.2 ± 32.0	3.1 ± 1.9	1.8 ± 0.7	96.6	1.8
NH_4-N	21.7 ± 11.9	8.4 ± 3.4	5.7 ± 1.7	73.8	3.0
KjN	22.7 ± 12.2	9.8 ± 2.6	7.7 ± 0.6	65.9	7.0
ortho-P	6.7 ± 3.3	1.6 ± 0.5	2.7 ± 0.5	59.6	1.0
TN	22.8 ± 11.1	12.0 ± 2.0	8.3 ± 0.7	63.8	3.6
TOC_t	31.9 ± 10.5	16.7 ± 2.1	15.2 ± 1.1	52.4	4.4
TOC_f	30.0 ± 9.2	16.0 ± 1.5	14.6 ± 0.9	51.2	7.5
HLR ($cm\ day^{-1}$)	18.7 ± 29.0 (min. 4.3–max. 101.7)				

Taking into account that the beds operation started more than four years ago and that the media consists of siliceous gravel with a low iron and calcium content, phosphorus removal also performs reasonably well. There are few signs of saturation of the sorption sites yet. The net production of phosphorus in the second bed suggests that there is some decay of organic material and/or a decrease in redox potential with subsequent P-release from Fe and Al complexes.

MODEL SETUP

For the model study of the Saxby treatment reed beds, the dynamic, compartmental model of Wynn and Liehr[4] was used as a starting point. This model describes carbon and nitrogen transformations in a HSCTW. Phosphorus transformations are not considered since these are mainly of physical-chemical nature and the main focus of the model is on microbial processes. This does imply that phosphorus concentrations are assumed to be non-limiting towards microbial and plant growth.

The model requires nine inputs: six regarding the influent (flow rate, BOD_t, organic N, NH_4-N, NO_3-N, and dissolved oxygen) and three regarding external influences (day length, air temperature, and precipitation). There are six standard outputs that are equal to the influent inputs. One can, however, also keep track of certain model variables such as plant growth, peat accumulation, evapotranspiration, and such, if that is of interest. The dynamics of the fifteen state variables are modelled via fifteen ordinary differential equations that contain a total of forty-two parameters related to physical, microbiological, and biological processes. Microbial reactions are represented by a standard Monod equation with switching functions, which means that biofilm processes and especially diffusion limitations are neglected. To counteract this rather drastic approach, one can lower the values of the microbial kinetic parameters. For a comprehensive explanation of the model, the reader is referred to the paper of Wynn and Liehr.[4]

One important assumption of the Wynn and Liehr[4] model is that the suspended solids removal efficiency approaches 100%, meaning that no particulate substances are leaving the reed bed. This was based on the fact that effluent SS levels of HSCTW generally are observed to be very low. For the Saxby case, effluent SS concentrations are not really negligible: they vary between 8 and 71 mg l^{-1} in the effluent of the first reed bed, and between 8 and 33 mg l^{-1} in the effluent of the second one. However, filtered TOC and N concentrations in the effluents were observed to be nearly equal to the total concentrations, thus the assumption that only dissolved carbon and nitrogen compounds are exiting the system is still valid.

Originally, the model was written in STELLA[7] code. The simulations for this study were carried out in WEST.[8] Since WEST works with the Model Specification Language (MSL), the model had to be recoded. During this phase, some minor model flaws were rectified.[9,10] Sub-surface flow is modelled by means of a classic Darcy equation. This concept was maintained although the following major adjustments were made to the water balance. Firstly, the effluent flow rate is now allowed to drop to zero if water loss by evapotranspiration exceeds the water supply as influent and precipitation. Secondly, several extra equations were added to make the model capable of dealing with flooding of the beds due to storm water peak discharges. This overland flow is modelled with a standard Manning equation to calculate flow rates dependent on bed slope, bed roughness, and water height.

To represent intermediate flow behavior, two completely mixed tanks in series were used to represent one reed bed. Unfortunately, no data from tracer tests were available to check this assumption, but the stability of the effluent concentrations (Fig. 2) seems to indicate a considerable degree of mixing. On the one hand, this lack of tracer test data adds to the uncertainty on the simulation results, but on the other hand, tracer test data will never be available during the design phase of a new reed bed for which purpose this model is being tested. The choice to use only two tanks in series was also based on the work of Wynn and Liehr[4] who obtained reasonable results with only one completely mixed tank to represent a reed bed with a higher L/W ratio. Finally, one should also consider that computation time increases as the model complexity increases.

One other important adjustment concerns the carbon balance. The original model of Wynn and Liehr[4] converts influent BOD data to dissolved organic carbon (DOC) and particulate organic carbon (POC) concentrations and vice versa for the effluent; the obvious advantage being that the model is able to use commonly available BOD concentrations. This conversion routine, however, uses several constants to translate oxygen demand into carbon concentrations, and to split total oxygen demand into dissolved and particulate fractions. In reality, these conversion values were observed to be highly variable and therefore of considerable influence on the model predictions. During this study, the model was therefore directly fed with DOC and POC data. Based on the observed relative stability of the ammonium effluent concentrations, the model was finally extended with a Freundlich sorption isotherm equation for ammonium, as described in McBride and Tanner.[11]

Obviously, this complexity of the model, as outlined in the previous paragraphs, enables us to better summarize the processes that occur within constructed treatment wetlands as well as to demonstrate interactions between certain components. It requires however estimation of fifteen initial conditions for the state variables and knowledge about or estimation of forty-two parameters, which is not a straightforward task. Rousseau et al.[3] demonstrated that simply copying parameter values from another model or another case study does not guarantee reliable model predictions. Extracting parameter values from literature data can also prove to be difficult due to a large variability in reported values. For example, values of one of the parameters applied in this model, i.e., the biomass oxygenation rate of *Phragmites australis* that represents root oxygen loss, are summarized by Brix.[12] Values are reported to vary between 0.02 and 12 g O_2 m^{-2} d^{-1}. Literature can thus give an indication of the possible range of parameter values, but often can not provide a crisp value. The following paragraphs therefore summarize the applied calibration routines based on the assembled input–output data and the resulting model fits.

GLOBAL SENSITIVITY ANALYSIS

Wynn and Liehr[4] carried out a basic sensitivity analysis of this model by visual comparison of the model outputs with the measured effluent concentrations, before and after having adjusted a parameter value. They found that the model was most sensitive toward changes in parameters that affect microbial growth and substrate use directly, i.e., heterotrophic maximum growth rate, heterotrophic death rate, and initial heterotrophic cell mass. Ammonium predictions where, as can be expected, significantly influenced by parameters controlling autotroph growth.

To quantify the model sensitivity and to identify the important parameters for further calibration, the method of van der Peijl and Verhoeven[13] was used for a global sensitivity analysis. This method examines the relative change in model output (X) divided by the relative change in the value of the parameter (Param) tested:

$$S_x = \frac{\delta X/X}{\delta \mathrm{Param}/\mathrm{Param}}$$

To judge this change in model output (X), the sum of squared errors (SSE) was used based on the deviations between the model predictions and the measured concentrations. The higher the absolute value of S_x, the more sensitive the model is toward changes of that parameter or in other words, a minor change of the parameter value causes a major change of the model predictions. S_x values were calculated for both reed beds, for DOC and NH_4 and for parameter changes of −25, −10, +10, and +25%. The results of the latter percent-wise parameter changes were fairly similar. The cut-off S_x value was arbitrarily set at 0.1.

In general, the reed bed dimensions proved to be highly sensitive parameters. This can be explained logically by the major impact of reed bed dimensions on the hydraulic residence time and thus on the water balance. Other sensitive parameters towards DOC and NH_4 predictions are summarised in Table 2.

Seemingly counterintuitive, the sensitivity analysis on the second reed bed revealed many more parameters with a high S_x value than the analysis on

Table 2: Results of the global sensitivity analysis: Parameters that have a major impact on DOC and NH_4 predictions for both reed beds (S_x value $\geq$ 0.1).

DOC–first reed bed
- Reed bed dimensions (L × W × d)
- Heterotrophic temperature factor (dimensionless)
- Hetrotrophic yield coefficient for NO_3 (g biomass (g NO_3-N)$^{-1}$)
- Heterotrophic maximum growth rate under aerobic conditions (d^{-1})
- Root oxygen loss (g O_2 m^{-2} d^{-1})
- Heterotrophic yield coefficient for dissolved oxygen (g biomass (g O_2)$^{-1}$)

NH_4—second reed bed
- Reed bed dimensions (L × W × d)
- Porosity
- Freundlich specific NH_4 sorption rate coefficient (d^{-1})
- Freundlich exponent (dimensionless) Freundlich solid-liquid NH_4 partition Coefficient (L (kg gravel)$^{-1}$)

DOC–second reed bed
- Same as bed 1+
- Hydraulic conductivity
- Porosity
- Autotrophic oxygen affinity constant (mg O_2 L^{-1})
- Microbial C content (g C (g biomass^1)
- Peat C content (g C (g peat)$^{-1}$) Heterotrophic affinity constant for organic material (mg L^{-1})
- Heterotrophic death rate (d^{-1})
- Heterotrophic oxygen affinity constant (mg O_2 L^{-1})
- Autotrophic temperature factor (dimensionless)
- Autotrophic maximum growth (d^{-1})
- Autotrophic yield coefficient for oxygen (g biomass (g O_2)$^{-1}$)
- Peat accumulation rate (g peat d^{-1})

NH_4—second reed bed
- Same as bed 1 +
- Hydraulic conductivity
- C:N ratio of reed plants (g C g N^{-1})
- C content of reed plants (g C (g biomass)$^{-1}$)
- Reed growth rate (g biomass m^{-2} d^{-1})

the first reed bed did. However, due to the low concentrations, other processes like for instance plant uptake become relatively more important and related parameters therefore become more sensitive.

The outcomes for DOC are generally in accordance with the findings of Wynn and Liehr:[4] microbial parameters are the more sensitive ones. However, when looking at the NH_4 transformation processes, the newly introduced Freundlich isotherm parameters prove to be the most sensitive ones.

MODEL CALIBRATION

Once the most sensitive parameters had been identified, their optimal value was determined by searching that value that results in the lowest SSE, or in other words the parameter value that results in a minimal deviation between measured and simulated concentrations. Two examples of the outcomes of this procedure are summarized in Figure 3 for the parameters biomass oxygenation rate and heterotrophic yield coefficient for dissolved oxygen.

Figure 3 clearly illustrates that the optimal parameter values can be different for every variable. For example, a biomass oxygenation rate of 0.22 g O_2 m^{-2} d^{-1} yields a best fit (minimal SSE) for DOC but not for NH_4, where a best fit is obtained with a biomass oxygenation rate value of 0.1 g O_2 m^{-2} d^{-1}. All optimal parameter values must, therefore, be taken into account when calibrating the model and a trade-off has to be made between the impacts on the different SSE values.

SIMULATION RESULTS

Figure 4 compares simulated and measured effluent concentrations of DOC and NH_4-N of the first reed bed at Saxby. These graphs show the best possible fit, obtained by introducing the optimal parameter values into the model, as identified in the previous paragraph. One can see that the DOC effluent concentrations fit very well, except for the two small peaks at day 3 and day 5, which

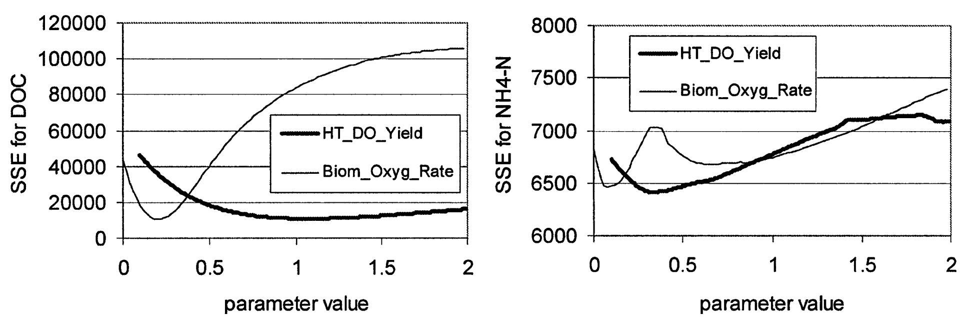

Figure 3: Impact of varying parameter values of the heterotrophic yield coefficient for dissolved oxygen (thick line) and the biomass oxygenation rate (thin line) on the model fits or SSEs for DOC and NH_4.

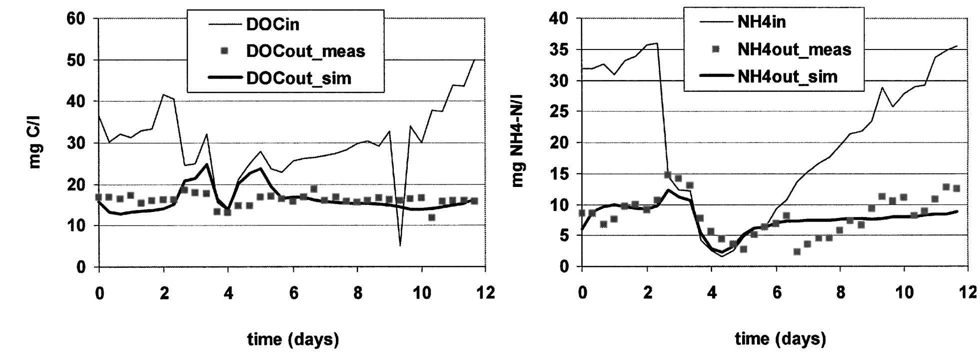

Figure 4: Left panel: Representation of measured influent and effluent DOC concentrations at the first reed bed at Saxby and comparison with simulated effluent DOC concentrations. Right panel: Representation of measured influent and effluent NH_4-N concentrations at the first reed bed at Saxby and comparison with simulated effluent NH_4-N concentrations.

coincide with the storm peak flow rates. The model seems to underestimate the buffering capacity of the reed bed. Simulated NH_4-N effluent concentrations on the contrary are less dynamic than was observed in reality.

For validation purposes, the model was run again with the dataset of the second reed bed. Especially, N removal was not adequately predicted. This does not immediately imply that the model is incorrect. Indeed, some parameters and initial conditions can be different for Bed 1 and Bed 2. Because plants and microorganisms in the second reed bed are subjected to smaller loads, several authors have proven that, e.g., growth rates are lower. Hence, new simulations with among others lower growth rates were performed and these gave somewhat better results. Figure 5 compares simulated and measured effluent concentrations of DOC and NH_4-N of the second reed bed at Saxby. These graphs

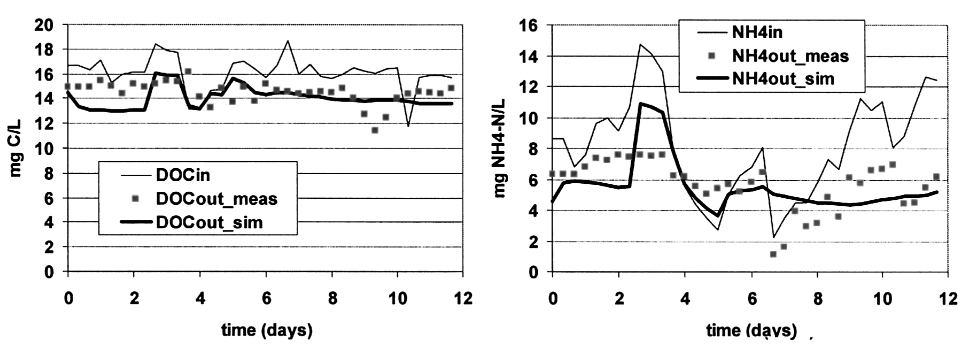

Figure 5: Left panel: Representation of measured influent and effluent DOC concentrations at the second reed bed at Saxby and comparison with simulated effluent DOC concentrations. Right panel: Representation of measured influent and effluent NH_4-N concentrations at the second reed bed at Saxby and comparison with simulated effluent NH_4-N concentrations.

show again the best possible fit, obtained by introducing the optimal parameter values into the model, as identified in the previous paragraph. Since for the second reed bed more parameters were found to be sensitive, obtaining a best fit was not obvious. Especially, the model predictions of NH_4 deviate considerably from the measured concentrations.

DISCUSSION

Although Wynn and Liehr[4] obtained fair results with their long-term, low-frequent dataset, the initial model results for the Saxby case were not satisfying at all. There are a number of possible causes for this discrepancy:

- *Time steps*: Wynn and Liehr[4] used a dataset that consisted of biweekly measurements of C and N components (grab samples). They interpolated between data points to have daily inputs for the model. This is totally unlike the Saxby dataset (eight-hour composite samples) and will certainly have some influence on the model performance.
- *Simulation period*: Wynn and Liehr[4] performed a simulation over almost one year and, thus, covered several seasons. This was not the case for the Saxby dataset (only summer conditions), and will again have some influence on the model output.
- *Model uncertainty*: It is quite possible that some processes occur in constructed treatment wetlands that are not included in the model. Due to external conditions, these processes might have been of minor importance in the Wynn and Liehr[4] case, but of bigger importance in the Saxby case.
- *Measurements*: Analytical uncertainties together with the use of noncooled samplers might have caused minor deviations between measured and actual concentrations.

One important conclusion was derived from preliminary simulations (data not shown) and the given model predictions: knowledge of the water balance and the hydraulic behavior or rather the degree of mixing, is of utmost importance for the model performance. Too few continuously stirred tank reactors (CSTRs) in series cause every concentration peak to be flattened out whereas too many CSTRs result in false peak concentrations and, from a practical point of view, also in an increased simulation time. When gathering datasets for calibration, a simultaneous tracer test should, therefore, be carried out.

Because the model output does not always closely match the measured dynamics of the effluent concentrations, it might still be unwise at this point to apply the model as a design tool. Indeed, when accepting a too stable model output, a reed bed designed according to these model specifications could in reality produce an effluent that exceeds the standards from time to time. On the other hand, when accepting a too dynamic model output, the dimensions of the reed bed would probably be increased during the design phase to make sure the effluent quality will be acceptable. This will result in unnecessarily high investment costs.

CONCLUSIONS

Design of horizontal subsurface flow constructed treatment wetlands is usually based on the well-known state-of-the-art k-C* model.[1] One important shortcoming of this black-box model is the oversimplification of reality, which results in a large uncertainty on the model predictions. Another drawback is the inability of the k-C* model to predict short-term effluent dynamics. A possible solution for these drawbacks could be the application of dynamic compartmental models.

With the dynamic model of Wynn and Liehr[4] as a starting point, a new model was developed that reflects the conditions of the test site, a two-stage horizontal subsurface flow constructed treatment wetland in Saxby (Leicestershire, UK). Several model extensions, especially the NH_4-sorption sub-model and the imitation of overland flow, significantly enhanced the model validity.

In the next phase, this new model was calibrated by means of a high-frequent dataset collected at the Saxby treatment wetlands. A quantitative sensitivity analysis revealed that reed bed dimensions had a major impact on all model predictions, which can be explained easily by the relation between the reed bed dimensions and the hydraulic behaviour. Heterotrophic kinetic parameters had most influence on the DOC predictions, whereas the parameters from the Freundlich sorption isotherm had a major impact on the NH_4-N predictions. By varying the values of these most sensitive parameters, a best fit was searched between the model outputs and the measured effluent concentrations. For optimal results, some parameters needed different values for the first and second reed bed. This can be explained logically by different governing conditions in both reed beds.

Final simulation results of both reed beds were acceptable but missed some of the dynamics observed in reality. When using this model as a design tool, this could result in a too conservative design if the model output is more dynamic than in reality, or an under-dimensioned reed bed in case of a more stable model output than occurs in reality. Further calibration and validation with other datasets is thus needed to improve the model predictions and to reduce the parameter uncertainty. Possible steps to improve the reliability of the model output are multiple. Firstly, it would be valuable to close the mass balances of carbon and nitrogen. Extra equations, and thus extra parameters, will therefore have to be added to the model, resulting on the one hand in a higher model complexity, but on the other one also in a higher model transparency. Secondly, new calibration efforts with data from other constructed treatment wetlands should consider the following recommendations: (1) always carry out a tracer test, (2) enhance the information content of the dataset by varying the loading rates and (3) try to take as many direct measurements of parameters and initial conditions as possible. Finally, to be really valid for use as a design tool, the model should also be tested for seasonality.

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