Special Section: Reactive Transport Modeling

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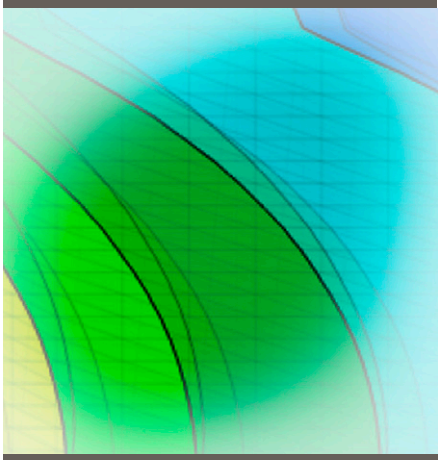

Two biokinetic models are presented for describing processes in constructed wetlands for wastewater treatment that are implemented in the HYDRUS software. Simulation results show the use of both kinetic models for horizontal flow constructed wetlands. Additionally, the importance of considering the effects of wetland plants is shown.

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Reactive Transport Modeling of Subsurface Flow Constructed Wetlands Using the HYDRUS Wetland Module

Constructed wetlands (CWs) are engineered water treatment systems designed to remove various types of contaminants. A large number of processes simultaneously contribute to water quality improvement in CWs. During the last decade, there has been a wide interest in the understanding of complex "constructed wetland" systems, including the development of numerical process-based models describing these systems. A number of process-based numerical models for subsurface flow (SSF) CWs have been developed during the last few years; however, most of them are either in an early stage of development or are available only in-house. The HYDRUS wetland module is the only implementation of a CW model that is currently publicly available. Version 2 of the HYDRUS wetland module includes two biokinetic model formulations simulating reactive transport in CWs: CW2D and CWM1. In CW2D, aerobic and anoxic transformation and degradation processes for organic matter, N, and P are considered, whereas in CWM1, aerobic, anoxic, and anaerobic processes for organic matter, N, and S are taken into account. We simulated horizontal flow CWs using both biokinetic models. Compared with the CWM1 implementation in the RETRASO code, the HYDRUS implementation was able to simulate fixed biomass, which is of high importance for obtaining realistic predictions for the treatment efficiency of CWs. We also compared simulation results for horizontal flow CWs obtained using both CW2D and CWM1 modules that showed that CWM1 produces more reasonable results because it also considers anaerobic degradation processes. The influence of wetland plants on the simulation results was also investigated. Simulated biomass profiles in the filter were completely different when considering O_2 release from roots, thus indicating the importance of considering plant effects.

Abbreviations: COD, chemical oxygen demand; CW, constructed wetland; HF, horizontal flow; SSF, subsurface flow; VF, vertical flow.

Constructed wetlands are systems that efficiently treat different types of polluted water. Constructed wetlands are engineered treatment systems that optimize treatment processes found in natural environments and are therefore considered to be sustainable, environmentally friendly solutions to engineering problems. Processes occurring in CWs are very complex and include a large number of simultaneously active physical, chemical, and biological processes that mutually influence each other (e.g., Kadlec and Wallace, 2009). For a long time, CWs have, therefore, been considered "black boxes," and little effort has been made to understand the main processes leading to the removal of contaminants.

During the last decade, models of different complexities have been developed for describing the processes in SSF CWs. The main objectives for numerical modeling of CWs are to obtain a better understanding of governing biological and chemical transformation and degradation processes, to provide insights into these "black box" systems, and to evaluate and improve existing design criteria (Langergraber, 2008, 2011).

No free water level is visible in SSF CWs, and water flows, either horizontally or vertically, through the porous filter media. Horizontal flow (HF) systems are often modeled by considering only saturated water flow conditions while the unsaturated zone is neglected. A series or network of continuously stirred tank reactors are most frequently used to describe the hydrodynamics of these systems, and reactions are modeled considering various complexities. When modeling vertical flow (VF) CWs with intermittent loading, consideration of transient, variably saturated flow conditions is essential and required. Due to the intermittent loading, these systems are highly dynamic, adding to the complexity

needed to model the overall system. Models applicable to VF CWs use either the Richards equation or various simplified approaches to describe variably saturated flow (Langergraber, 2011).

Only a few process-based numerical models have been developed that are capable of modeling reactive transport in both HF and VF CWs. According to Langergraber (2011), there are only three tools that have been designed to describe the transformation and degradation processes of wastewater pollutants in CWs, i.e., the HYDRUS wetland module (Langergraber and Šimůnek, 2006, 2011), PHWAT (Brovelli et al., 2009a, 2009b), and RETRASO (Ojeda et al., 2008; Llorens et al., 2011a, 2011b). Additionally, there is a tool for modeling only organic matter removal and O_2 transport (Wanko et al., 2006) and a biokinetic model implemented in MIN3P that describes processes involved in the remediation of contaminated groundwater (Maier et al., 2009; De Biase et al., 2011). Similarly to Wanko et al. (2006), Forquet et al. (2009) and Petitjean et al. (2011) also modeled diphasic transfer of O_2 in VF beds.

In this study, we used Version 2 of the HYDRUS wetland module. Version 2 includes two biokinetic model formulations: (i) the CW2D module (Langergraber and Šimůnek, 2005), and (ii) the CWM1 (Constructed Wetland Model 1) (Langergraber et al., 2009b). In CW2D, aerobic and anoxic transformation and degradation processes for organic matter, N, and P are taken into account, whereas in CWM1, aerobic, anoxic, and anaerobic processes for organic matter, N, and S are considered. The CWM1 model was developed with the main goal of providing a widely accepted model formulation for biochemical transformation and degradation processes in SSF CWs. The HYDRUS wetland module is the only implementation of a CW model that is currently commercially available to the public.

The HYDRUS Wetland Module

Principles

As described by Langergraber et al. (2009b), a number of submodels are required to simulate a SSF CW. These submodels include:

1. the water flow model, describing water flow in the porous media is of utmost importance,
2. the transport model, describing transport of constituents, as well as adsorption and desorption processes,
3. the biokinetic model, describing biochemical transformation and degradation processes,
4. the plant model, describing processes such as growth, decay, decomposition, nutrient uptake, and root O_2 release, and
5. the clogging model, describing clogging processes, i.e., transport and deposition of suspended particulate matter and bacterial and plant growth that may reduce the hydraulic capacity or conductivity of the filter medium.

Table 1. Principles of the CW2D and CWM1 biokinetic models (numbers in parentheses give the number of processes or components).

Principle	CW2D	CWM1
Processes	aerobic and anoxic (9)	aerobic, anoxic, and anaerobic (17)
Components	O_2, organic matter, N, and P (12)	O_2, organic matter, N, and S (16)

Most of the submodels required for a complete wetland model, with the exception of the clogging model and some processes of the plant model, are available in HYDRUS. The standard version of HYDRUS numerically solves the Richards equation for saturated–unsaturated water flow and the convection–dispersion equation for heat and solute transport. The flow equation incorporates a sink term to account for water uptake by plant roots. The solute transport equations consider convective–dispersive transport in the liquid phase, diffusion in the gaseous phase, as well as nonlinear nonequilibrium reactions between the solid and liquid phases (Šimůnek et al., 2011).

The biochemical transformation and degradation processes are described by the HYDRUS wetland module. In Version 2 of the HYDRUS wetland module, two biokinetic models simulating the transformation and degradation processes are implemented. Table 1 compares the principles of CW2D and CWM1.

1. The CW2D model (Langergraber and Šimůnek, 2005) was mainly developed for modeling VF systems and therefore includes only aerobic and anoxic transformation and degradation processes. These processes are described for the main constituents of wastewater, i.e., organic matter, N, and P.
2. The CWM1 model (Langergraber et al., 2009b) was developed as a general model that describes biochemical transformation and degradation processes for organic matter, N, and S in both HF and VF CWs. The CWM1 model describes all relevant aerobic, anoxic, and anaerobic biokinetic processes occurring in HF and VF CWs and required to predict effluent concentrations of organic matter, N, and S.

The influence of plants can be partly simulated using HYDRUS as well. Langergraber (2005) investigated the plant uptake models provided by HYDRUS (i.e., passive nutrient uptake coupled with water uptake) and concluded that it was possible to simulate plant uptake in high-loaded systems, e.g., systems treating mechanically pretreated municipal wastewater. For low-strength wastewater, the simulation results indicate that potential nutrient uptake is overestimated using these models. Oxygen release via roots can be modeled in a way similar to nutrient uptake (Toscano et al., 2009). It is not possible, however, to simulate growth, decay, and decomposition of the wetland plants using HYDRUS. For more details on the mathematical formulations used to model uptake

of water and solutes by plant roots, we refer to Šimůnek and Hopmans (2009), who described in detail the considered approach, and to the HYDRUS technical manual (Šimůnek et al., 2011).

It is also not possible to simulate transport and deposition of suspended particulate matter and their influence on the hydraulic conductivity. This would be of importance for long-term simulations that aim to predict the changes in long-term treatment performance and, finally, the failure of SSF CWs due to clogging (Langergraber et al., 2009a). In HYDRUS, suspended particulate matter compounds have to be considered as solute compounds.

The Gujer Matrix Representation of Biokinetic Models

It is common practice to present biokinetic models using the matrix notation introduced by the International Water Association for activated sludge models (Henze et al., 2000). The so-called Gujer matrix consists of three parts, representing (i) stoichiometry, (ii) kinetic rate expressions, and (iii) composition. A simple model representing aerobic heterotrophic bacteria growth and decay (adapted from Henze et al., 2000) was chosen as an example to illustrate the use of the Gujer matrix. Table 2 describes two processes (growth and decay of heterotrophic bacteria) and three components (biomass, substrate, and dissolved O_2). Bacteria need energy to integrate their C substrate and produce new biomass. Heterotrophs (X_{OHO}) find their energy and their C source in an organic substrate (S_B) and use dissolved O_2 (S_{O2}) as an electron acceptor under aerobic conditions. Consequently, only part of the substrate used by bacteria will directly contribute to biomass growth ($1/Y_{OHO}$), whereas the other part is oxidized to produce energy ($1 - 1/Y_{OHO}$).

In this example, the growth rate depends on the maximum growth rate of the heterotrophic biomass ($\mu_{OHO,max}$), the biomass concentration (X_{OHO}), the availability of the substrate to the bacteria ($S_B/(K_{SB,OHO} + S_B)$, where $K_{SB,OHO}$ is the half-saturation coefficient for S_B), and the availability of electron acceptors ($S_{O2}/(K_{SO2,OHO} + S_{O2})$, where $K_{SO2,OHO}$ is the half-saturation coefficient for S_{O2}). The ratios $S_B/(K_{SB,OHO} + S_B)$ and $S_{O2}/(K_{SO2,OHO} + S_{O2})$ are the Monod-type equations that are used in this model formulation as switching functions for substrate, nutrients, alkalinity, electron acceptors, and other components. Similarly, when a process occurs only when a component is absent (e.g., dissolved O_2 in anoxic processes), the switching function takes the following form: $K_{O2,OHO}/(K_{O2,OHO} + S_{O2})$.

Table 2. Gujer matrix describing process kinetics and stoichiometry for heterotrophic bacterial growth in an aerobic environment (adapted from Henze et al. (2000), using the notations of Corominas et al., 2010). Stoichiometric parameters: Y_{OHO}, heterotrophic yield coefficient; kinetic parameters: $\mu_{OHO,max}$, maximum heterotrophic growth rate; $K_{SB,OHO}$, half-saturation coefficient for substrate; $K_{SO2,OHO}$, half-saturation coefficient for O_2; b_{OHO}, heterotrophic decay rate.

Mass balance ↓	→ Continuity	Heterotrophic biomass (mg COD L^{-1})	Substrate (mg COD L^{-1})	Dissolved O_2 (mg COD L^{-1})	
	Component (i)	1	2	3	Process rate ρ_j
	Process (j)	X_{OHO}	S_B	S_{O2}	
	1. Growth	1	$-1/Y_{OHO}$	$-(1 - Y_{OHO})/Y_{OHO}$	$\mu_{OHO,max}[S_B/(K_{SB,OHO} + S_B)] \times [S_{O2}/(K_{SO2,OHO} + S_{O2})]X_{OHO}$
	2. Decay	−1		−1	$b_{OHO} X_{OHO}$

The continuity check for every process is calculated by multiplying the stoichiometric coefficients by the corresponding term in the composition matrix for every component and summing up for different processes (because O_2 is negative chemical O_2 demand [COD], its coefficient must therefore be multiplied by −1).

Reaction rates for the three components discussed above are calculated by summing up products of stoichiometric factors and process rates for the different processes involved. For example, reaction rates for heterotrophic biomass (r_{XOHO}), organic substrate (r_{SB}), and O_2 (r_{SO}) are calculated as follows:

$$
\begin{aligned}
r_{X_{OHO}} &= \mu_{OHO,max} \frac{S_B}{K_{S_B,OHO} + S_B} \frac{S_{O_2}}{K_{S_{O_2},OHO} + S_{O_2}} \times X_{OHO} \\
&\quad - b_{OHO} X_{OHO} \\
r_{S_B} &= -\frac{1}{Y_{OHO}} \mu_{OHO,max} \frac{S_B}{K_{S_B,OHO} + S_B} \\
&\quad \times \frac{S_{O_2}}{K_{S_{O_2},OHO} + S_{O_2}} X_{OHO} \\
r_{S_O} &= -\left(\frac{1 - Y_{OHO}}{Y_{OHO}}\right) \mu_{OHO,max} \\
&\quad \times \frac{S_B}{K_{S_B,OHO} + S_B} \frac{S_{O_2}}{K_{S_{O_2},OHO} + S_{O_2}} \times X_{OHO} \\
&\quad - b_{OHO} X_{OHO}
\end{aligned}
\qquad [1]
$$

The CW2D and CWM1 Biokinetic Models

Table 3 compares the components defined in the CW2D and CWM1 model formulations. For detailed information about the CW2D and CWM1 biokinetic models, as well as their parameter values, see the original studies, i.e., Langergraber and Šimůnek (2005) and Langergraber et al. (2009b), respectively. As described above, both biokinetic models consider processes affecting organic matter and N. Additionally, CW2D considers processes affecting P, whereas CWM1 considers processes affecting S. It is assumed that all components except bacteria are soluble (including the particulate COD fraction) and that bacteria are immobile. Organic N (in CW2D and CWM1) and organic P (in CW2D) are modeled as part of the COD. Note that because wastewater constituents considered in the CW2D and CWM1 biokinetic models are

Table 3. Comparison of CW2D (Langergraber and Šimůnek, 2005) and CWM1 (Langergraber et al., 2009b) components.

CW2D: organic matter, N, P	CWM1: organic matter, N, S
CW2D components 1. SO: dissolved O_2 2. CR: readily biodegradable soluble chemical oxygen demand (COD) 3. CS: slowly biodegradable soluble COD 4. CI: inert soluble COD 5. XH: heterotrophic bacteria 6. XANs: autotrophic NH_4–oxidizing bacteria (*Nitrosomonas* spp.) 7. XANb: autotrophic NO_2–oxidizing bacteria (*Nitrobacter* spp.) 8. NH4N: NH_4–N and NH_3–N 9. NO2N: NO_2–N 10. NO3N: NO_3–N 11. N2: elemental N_2 12. PO4P: PO_4–P Additional component (in the HYDRUS implementation) 13. nonreactive tracer Nitrification is modeled as a two-step process	Soluble components 1. SO: dissolved O_2 2. SF: fermentable, readily biodegradable soluble COD 3. SA: fermentation products as acetate 4. SI: inert soluble COD 5. SNH: NH_4–N and NH_3–N 6. SNO: NO_3–N and NO_2–N 7. SSO4: SO_4–S 8. SH2S: H_2S-S Particulate components 9. XS: slowly biodegradable particulate COD 10. XI: inert particulate COD 11. XH: heterotrophic bacteria 12. XA: autotrophic nitrifying bacteria 13. XFB: fermenting bacteria 14. XAMB: acetotrophic methanogenic bacteria 15. XASRB: acetotrophic SO_4-reducing bacteria 16. XSOB: S^{2-}–oxidizing bacteria Additional component (in the HYDRUS implementation) 17. nonreactive tracer

Table 4. Components of CW2D and CWM1 in the liquid (L) and solid (S) phases. See Table 3 for component definitions.

Component	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
CW2D	L	L+S	L+S	L+S	S	S	S	L+S	L	L	L	L+S	L+S	–	–	–	–
CWM1	L	L+S	L+S	L+S	L+S	L	L	L	L+S	L+S	S	S	S	S	S	S	L+S

different, there is no direct conversion between the two model components. Component symbols (e.g., SO for dissolved O_2), as defined in Table 3, are used throughout the text and in figures and tables when referring to various chemicals and bacterial groups.

Table 4 summarizes in what phase (i.e., liquid or solid or both) the CW2D and CWM1 components are defined. For components defined in both phases (L + S), adsorption and desorption processes can be considered. As mentioned above, suspended particulate organic matter compounds, i.e., slowly biodegradable (XS) and inert (XI) particulate COD in CWM1, are considered as solute compounds. Note that the number of components in Table 4 is increased by one compared with that given in Table 3 for both CW2D and CWM1. In both models, a nonreactive tracer that is independent of other components and that can be used to derive the hydraulic retention time is added in the HYDRUS wetland module. This nonreactive tracer is defined in both liquid and solid phases (Langergraber and Šimůnek, 2011).

Table 5 compares the processes defined in the CW2D and CWM1 model formulations. Only aerobic and anoxic processes are defined in CW2D. Two main types of bacteria, i.e., heterotrophic and autotrophic bacteria, are considered. One special feature of CW2D is that nitrification is modeled as a two-step process, i.e., from NH_3 via NO_2 to NO_3. Because anaerobic processes are additionally defined in CWM1, six different types of bacteria need to be considered in this model. In addition to heterotrophic and autotrophic bacteria, fermenting, acetotrophic methanogenic, acetotrophic SO_4–reducing, and S^{2-}–oxidizing bacteria are also considered to account for the main anaerobic processes.

For detailed information on additional model equations (e.g., oxygen re-aeration) and on how to set up models for SSF CWs in HYDRUS, see the manuals for the HYDRUS wetland module (Langergraber and Šimůnek, 2006, 2011). For more general information about the HYDRUS family of codes, see Šimůnek et al. (2008), and for detailed information about the software (such as governing equations for water flow, solute transport, adsorption–desorption processes, the plant uptake model, and boundary conditions), see the HYDRUS technical manual (Šimůnek et al., 2011).

Simulation Results

Numerical Verification of Biokinetic Model Implementation

Our numerical verification focused on the two biochemical models. The water flow and solute transport parts of the HYDRUS model are widely used and generally accepted to be verified (Šimůnek et al., 2008).

Table 5. Comparison of CW2D (Langergraber and Šimůnek, 2005) and CWM1 (Langergraber et al., 2009b) processes. See Table 3 for component definitions.

CW2D	CWM1
Heterotrophic bacteria: 1. Hydrolysis: conversion of CS into CR. 2. Aerobic growth of XH on CR (mineralization of organic matter). 3. Anoxic growth of XH on CR (denitrification on NO2N). 4. Anoxic growth of XH on CR (denitrification on NO3N). 5. Lysis of XH. Autotrophic bacteria: 6. Aerobic growth of XANs on SNH (ammonium oxidation). 7. Lysis of XANs. 8. Aerobic growth of XANb on SNH (nitrite oxidation). 9. Lysis of XANb.	Heterotrophic bacteria: 1. Hydrolysis: conversion of XS into SF. 2. Aerobic growth of XH on SF (mineralization of organic matter). 3. Aerobic growth of XH on SA (mineralization of organic matter). 4. Anoxic growth of XH on SF (denitrification). 5. Anoxic growth of XH on SA (denitrification). 6. Lysis of XH. Autotrophic bacteria: 7. Aerobic growth of XA on SNH (nitrification). 8. Lysis of XA. Fermenting bacteria: 9. Growth of XFB (fermentation). 10. Lysis of XFB. Acetotrophic methanogenic bacteria: 11. Growth of XAMB: Anaerobic growth of acetotrophic, methanogenic bacteria XAMB on acetate SA. 12. Lysis of XAMB. Acetotrophic sulphate reducing bacteria: 13. Growth of XASRB: Anaerobic growth of acetotrophic, sulphate reducing bacteria. 14. Lysis of XASRB. Sulphide oxidizing bacteria: 15. Aerobic growth of XSOB on SH2S: The opposite process to process 13, the oxidation of SH2S to SSO4. 16. Anoxic growth of XSOB on SH2S: Similar to process 15 but under anoxic conditions. 17. Lysis of XSOB.

To numerically verify the implementation of the two biokinetic models, the reactions involving organic matter were evaluated using a simple example. Due to different components and processes considered by the CW2D and CWM1 models, no more complex verification of the model implementation could be made.

In this simple example, it was assumed that only heterotrophic bacteria (XH) were present, i.e., that only processes of hydrolysis, mineralization of organic matter, and lysis of XH took place. Initial concentrations were set, for CW2D, to 1 mg L^{-1} dissolved O_2 (SO), 1 mg L^{-1} readily biodegradable soluble COD (CR), 10 mg L^{-1} slowly biodegradable soluble COD (CS), 10 mg kg^{-1} XH, and 1 mg L^{-1} PO_4–P, and for CWM1, 1 mg L^{-1} SO, 1 mg L^{-1} fermentable, readily biodegradable soluble COD (SF), 10 mg L^{-1} slowly biodegradable particulate COD (XS), and 10 mg kg^{-1} XH. Initial PO_4–P concentrations were set to values larger than zero to prevent inhibition of processes due to the lack of P, which is required as a nutrient. Initial concentrations for all other components were zero (including initial concentrations for N components—note that NH_3 is released during hydrolysis and then utilized by bacteria during growth). For the numerical verification, we chose to use low concentrations to verify a greater number of processes. For example, having high initial NH_3 concentrations would prevent us from detecting the very low release of N during hydrolysis.

A vertical domain of 20 by 20 cm was discretized into three columns and 21 rows. This resulted in a two-dimensional finite element mesh consisting of 63 nodes and 80 triangular finite elements. No flow was considered into or out of the domain. Default HYDRUS soil hydraulic parameters (as per the van Genuchten–Mualem model with no hysteresis; see Šimůnek et al., 2011) for sand were used. Sand was chosen in this example because it is commonly used as a filter material in VF CWs. The water table was set to be 8 cm above the bottom boundary and the simulations were run for 1 d.

Figure 1 shows the simulation results for an observation node located 2 cm above the water table. The location above the water table was chosen to compare aerobic processes implemented in CW2D and CWM1 because different processes occur below the water table after O_2 is consumed (note that anaerobic processes are implemented in CWM1). The volumetric water content at this observation node was 42%. Figure 1 shows that the same results could be obtained using both biokinetic models. The

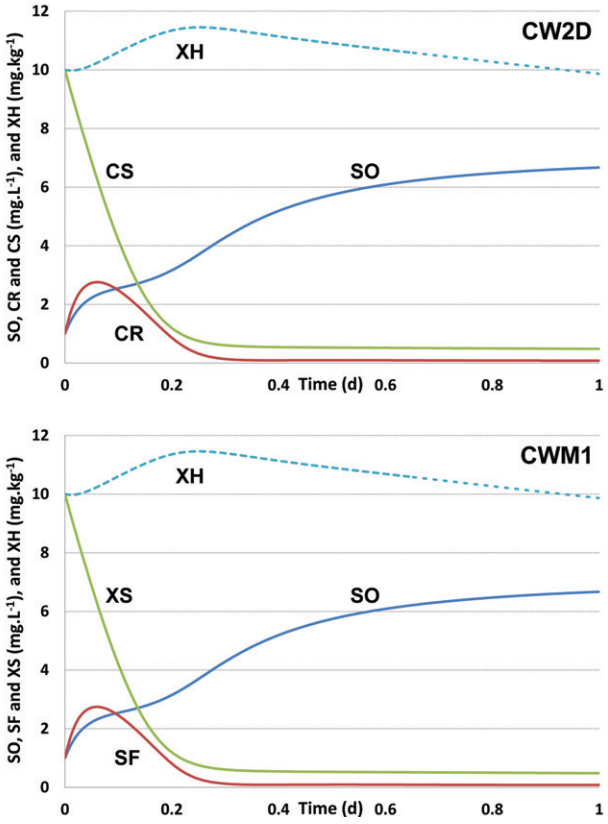

Fig. 1. Simulation results obtained for an observation node located 2 cm above the water table for dissolved O_2 (SO), readily biodegradable soluble chemical O_2 demand (COD) (CR), slowly biodegradable soluble COD (CS), and heterotrophic bacteria (XH) using the CW2D model (top) and for SO, fermentable, readily biodegradable soluble COD (SF), slowly biodegradable particulate COD (XS), and XH using the CWM1 model (bottom).

slowly biodegradable COD (CS in CW2D and XS in CWM1) is hydrolyzed, while readily biodegradable COD (CR in CW2D and SF in CWM1) is produced. The readily biodegradable COD is then mineralized (i.e., converted into CO_2 and H_2O) due to aerobic growth of XH. Once the readily biodegradable COD is used up, bacteria start dying at a constant rate. During this lysis process, bacteria are decomposed into the slowly biodegradable organic matter and a release of inert organic matter and NH_3 takes place (not shown in Fig. 1). At the end of the 1-d simulation, the NH_3–N and inert organic matter concentrations at the observation node were 0.36 and 0.31 mg L^{-1}, respectively.

This simple example shows that both biokinetic models have been implemented correctly in the HYDRUS wetland module. Due to different components and processes considered by the CW2D and CWM1 models, no more complex comparison of the model implementations could be made.

Comparison of Results Obtained Using the Implementation of CWM1 into HYDRUS and RETRASO

Llorens et al. (2011a, 2011b) implemented CWM1 into the RETRASO code. The CWM1-RETRASO code is based on the two-dimensional finite-element code, RetrasoCodeBright (RCB), which simulates reactive transport of dissolved and gaseous species for nonisothermal saturated or unsaturated flow domains. In RCB, the first module calculates the flow variables and passes them to the second module, which calculates the reactive transport (Rezaei et al., 2005; Saaltink et al., 2003).

Llorens et al. (2011b) simulated, as a test case, a HF bed with a length of 10.3 m and a width of 5.3 m. The water level in the bed was 0.5 m. The first 0.3 m of the bed, the mixing zone, was filled with coarse gravel. Llorens et al. (2011b) simulated only the main layer of the bed (with a length of 10 m filled with gravel with a d_{60} of 10 mm and porosity of 41%), whereas our HYDRUS implementation considered the mixing zone as well (the red circle in Fig. 2B). Figure 2B also shows a typical flow path in a HF bed.

In the HYDRUS implementation, the vertical domain of 10.3 and 0.6 m was discretized into 33 columns and 23 rows, resulting in a two-dimensional finite-element mesh consisting of 805 nodes and 1496 triangular finite elements. An atmospheric boundary condition with a water flux of 2.1 m d^{-1} to represent wastewater loading was applied at the top of the mixing zone, whereas the effluent boundary was represented using a constant-head boundary condition (0.5 m) at the bottom of the right end of the bed. Due to the lack of data about the mixing zone, the same material parameters as for the main zone were used. Initial concentrations of 1 mg L^{-1} were assigned for all solute compounds. Initial concentrations for bacteria were set to 1 mg kg^{-1} for all nodes below the water table and zero above. Various simulations with HYDRUS were run for 50 d.

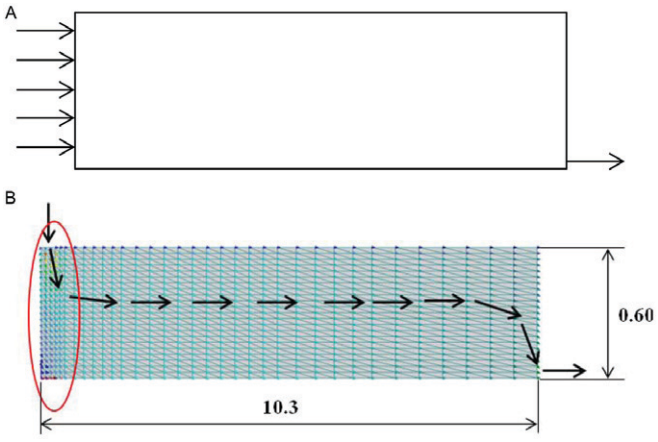

Fig. 2. Implementation of the horizontal flow bed in RETRASO (top, Llorens et al., 2011b) and HYDRUS (bottom, dimensions in meters). The red circle indicates the mixing zone.

Llorens et al. (2011b) defined several influent scenarios to test their implementation. For our comparison, we used the scenario in which the HF bed is loaded with 20 mm d^{-1} of wastewater, with only dissolved O_2 (SO) and slowly biodegradable COD (XS) present in the influent (Scenario 3 of Llorens et al., 2011b). The influent concentrations were 0.86 and 115 mg O_2 L^{-1} for SO and XS, respectively. In the HYDRUS simulations, influent concentrations of bacteria were zero, while in the RETRASO simulations, constant influent concentrations of bacteria were considered. This was necessary because the RETRASO code does not consider a fixed biomass. Bacteria were assumed to be transported through the filter similarly to solute components. Therefore, the initial concentrations of bacteria were assumed by Llorens et al. (2011b) to be the same as in the influent.

Figure 3 shows the concentration profiles of fermentable, readily biodegradable soluble COD (SF), fermentation products as acetate (SA), and XS along the flow path simulated using RETRASO (Llorens et al., 2011b). The XS is converted into SF by hydrolysis and further used for the growth of heterotrophic bacteria (XH). The maximum concentration of SF was simulated to be around 70 mg O_2 L^{-1}. Due to fermentation and microbial lysis, acetate is built up along the flow path in the HF bed.

Figure 4 shows the concentration profiles of SF, SA, and XS after the 50-d simulation time using the CWM1 module of HYDRUS. The same values for the biokinetic model parameters as reported by Llorens et al. (2011b) were used for these simulations. The left side of Fig. 5 presents the corresponding concentration profiles of heterotrophic (XH), autotrophic nitrifying (XA), fermenting (XFB), and acetotrophic methanogenic (XAMB) bacteria. It can be clearly seen in Fig. 5 that the bacteria concentration profiles are far from those simulated by Llorens et al. (2011b). Consequently, the concentration profiles of solute compounds shown in Fig. 4 are different from those presented in Fig. 3. A rapid transformation of XS into SF by hydrolysis takes place near the inlet, due to high bacteria concentrations there. Under anaerobic conditions, SF is further converted into SA by fermenting bacteria (XFB). Contrary to the RETRASO results (Fig. 3), SA is fully degraded before it reaches the effluent (Fig. 4). In this specific example with only XS in the influent, all degradable COD is removed within about half of the flow distance in the HF bed (Fig. 4). Aerobic conditions occur at the end of the HF bed and therefore all degradable COD produced by lysis processes is mineralized as well.

The concentration of SF is almost constant in the HF bed. In this scenario, the influent consists of only XS, which is anaerobically converted to SA, with SF being only an intermittent product. The almost constant value of SF of about 1.5 mg L^{-1} (Fig. 4) is caused by the rather high saturation coefficient for SF in the fermentation process.

Concentrations of XH and XFB are highest near the water table (Fig. 5). After the organic matter is degraded, O_2 diffuses into deeper zones of the bed and heterotrophic bacteria can also grow in these deeper zones (about 7 m away from the inflow in Fig. 5). Although no free NH_3 is introduced in the influent, NH_3 is produced inside of the HF bed during degradation of the organic matter and lysis of bacteria. Nitrifying bacteria (XA) grow in locations where NH_3 is available, the organic matter is already removed, and O_2 is thus available for nitrification. Acetotrophic methanogenic bacteria (XAMB) grow on acetate (SA) under anaerobic conditions.

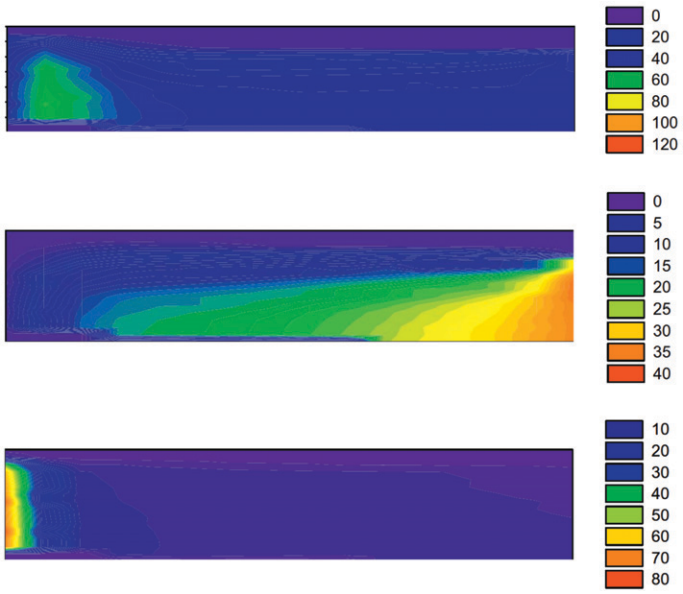

Fig. 3. Concentration profiles (mg L^{-1}) of fermentable, readily biodegradable soluble chemical oxygen demand (COD) (SF) (top), fermentation products as acetate (SA) (middle), and slowly biodegradable particulate COD (XS) (bottom) for Scenario 3 of Llorens et al. (2011b) simulated using the CWM1 implementation in RETRASO (adapted from Llorens et al., 2011b). Dimensions of the transport domain in RETRASO are 10.0 by 0.7 m.

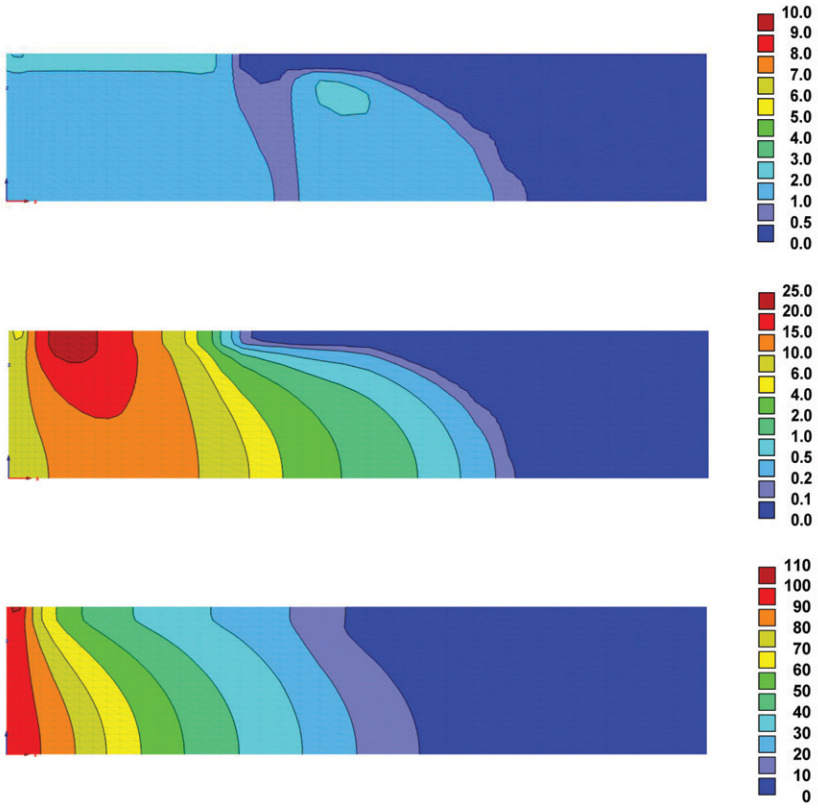

Fig. 4. Concentration profiles (mg L^{-1}) of fermentable, readily biodegradable soluble chemical oxygen demand (COD) (SF) (top), fermentation products as acetate (SA) (middle), and slowly biodegradable particulate COD (XS) (bottom) simulated with HYDRUS using the CWM1 biokinetic model. Dimensions of the transport domain in HYDRUS are 10.3 by 0.6 m.

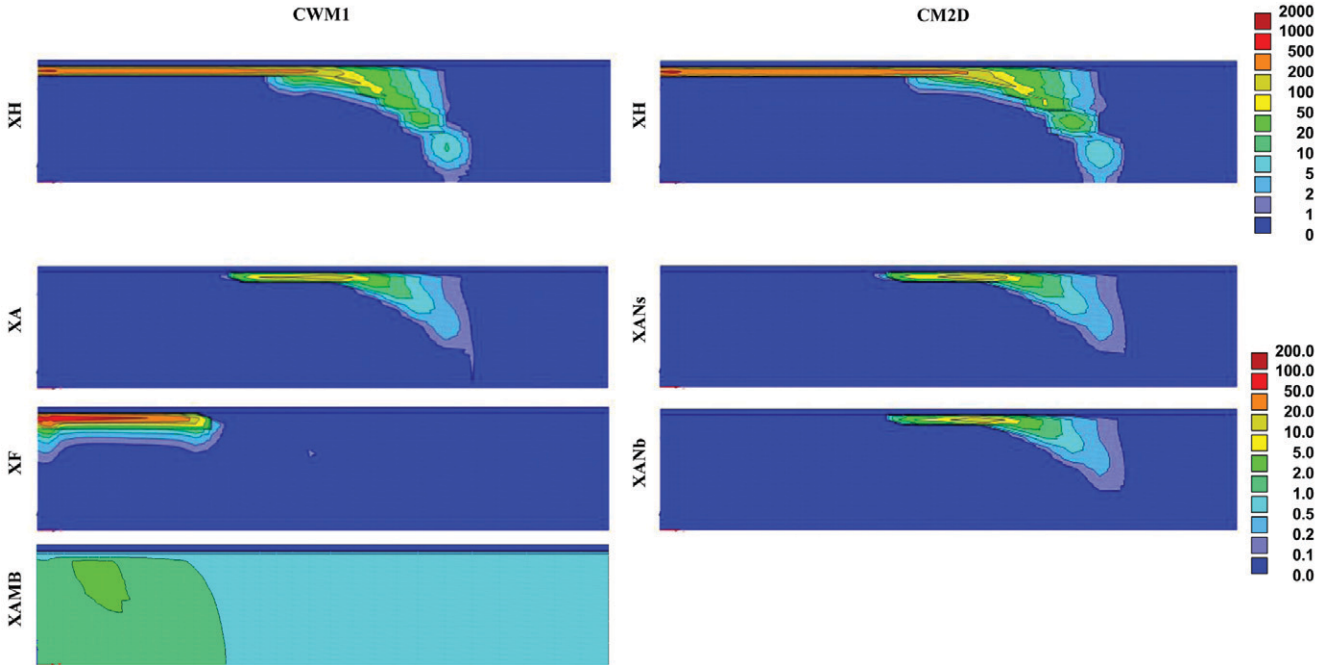

Fig. 5. Bacteria concentration profiles (mg kg^{-1}) simulated with HYDRUS using the CWM1 (left) and CW2D (right) biokinetic models. Left (from top to bottom): heterotrophic bacteria (XH), autotrophic nitrifying bacteria (XA), fermenting bacteria (XFB), and acetotrophic methanogenic bacteria (XAMB); right (from top to bottom): heterotrophic bacteria (XH), autotrophic NH_4–oxidizing bacteria (XANs), and autotrophic NO_2–oxidizing bacteria (XANb).

Simulated XAMB concentrations are lower after 50 d because they grow more slowly than the other bacteria types.

Comparison of the CWM1 and CW2D Models for Simulating Horizontal Flow Beds

The aim of this example is to compare simulation results for the same CW system obtained with the two biokinetic models, i.e., CWM1 and CW2D. The same setup as described above was also used for simulations with the CW2D biokinetic model. Again, the influent concentrations were 0.86 and 115 mg O_2 L^{-1} for SO and slowly biodegradable COD (CS in CW2D), respectively. Because no anaerobic processes are considered in CW2D, hydrolysis of CS produces the readily biodegradable COD (CR), which is consumed by heterotrophic bacteria (XH). Contrary to CWM1 (Fig. 4), a buildup of readily biodegradable COD is simulated by CW2D (Fig. 6). Concentration profiles of heterotrophic bacteria (XH) and autotrophic bacteria (XANs and XANb), as shown in Fig. 5 (right), were similar to those for XH and XA predicted using CWM1 (Fig. 5, left). As shown in Fig. 5, both biokinetic models predict aerobic bacteria growth also in deeper depths of the HF bed, at about 75% of the flow distance. This can be explained by the fact that all organic matter is consumed by this point and O_2 can diffuse into deeper zones of the HF bed, facilitating aerobic processes.

The concentration profiles for slowly biodegradable COD (XS) in Fig. 4 and (CS) in Fig. 6 look almost the same, although CWM1 considers acetotrophic methanogenic bacteria (XAMB), from which one would expect an additional removal of the organic matter. This can be explained by the fact that XAMB grows very slowly and a longer simulation time (e.g., 1 yr) would be needed to establish significant XAMB concentrations in the HF bed; however, we did not do calculations for time periods of 1 yr or longer in this example.

Figure 7 shows the concentration profiles of NH_3 and NO_3 simulated using CWM1 and CW2D. The concentrations of all N compounds are low because no N was in the influent and all N was released only during hydrolysis. The amounts of built-up NH_3 as well as the final NO_3 concentrations in the effluent of the HF bed are similar for both biokinetic models. The NO_3 profiles differ a little in the zones where nitrification occurs. This can be explained by different nitrification models in CW2D and CWM1, which are modeled as a two-step and a one-step process, respectively. In CW2D, where nitrification is modeled as a two-step process, only low concentrations of NO_2 occur (Fig. 8), indicating that there is enough O_2 available for the second nitrification step.

Considering the Influence of Plants in Wetlands

With the aim of evaluating the influence of wetland plants on the removal of contaminants in HF beds, the HF bed of Llorens et al. (2011b) that we described above was used. In these new simulations, the HF bed was loaded with wastewater with a hydraulic loading rate of 36 mm d^{-1}. The influent concentrations used for the CWM1 and CW2D simulations were (see Table 3 for definitions): CWM1 components (in mg L^{-1}): SO, 0.86; SF, 170; SA, 27; SI, 13; SNH, 57; SNO, 0; SSO4, 33; SH2S, 0; XS, 33; and XI, 13; CW2D components (in mg L^{-1}): SO, 0.86; CR, 197; CS, 33; CI, 26; NH4N, 57; NO2N, 0; NO3N, 0; N2N, 0; and PO4P, 10. The CWM1 influent concentrations were the same as those used in Scenario 5 of Llorens et al. (2011b), while the CW2D influent concentrations were calculated from the CWM1 influent concentrations (CR = SF + SA, CS = XS, and CI = SI + XI). In the CW2D simulations, PO_4–P was considered in the inflow, whereas S was not considered.

Figure 9 shows the spatial distribution of root water uptake in the vertical domain. As reported by Headley et al. (2005), root

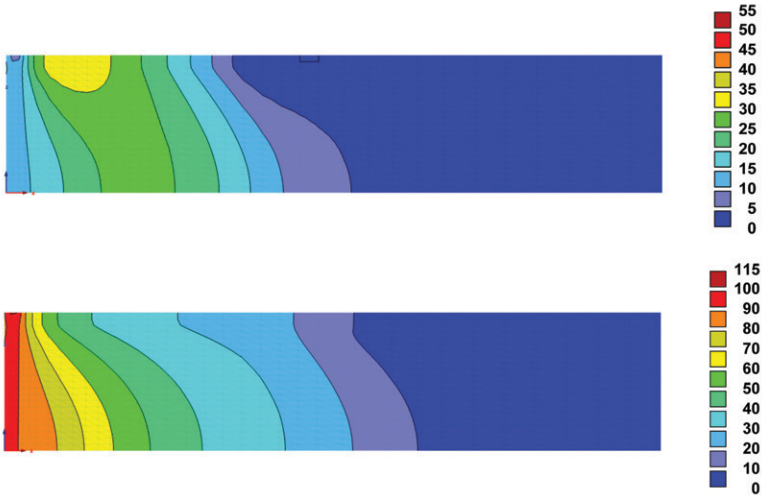

Fig. 6. Concentration profiles (mg L^{-1}) of readily biodegradable soluble chemical oxygen demand (COD) (CR) (top) and slowly biodegradable soluble COD (CS) (bottom) simulated with HYDRUS using the CW2D biokinetic model.

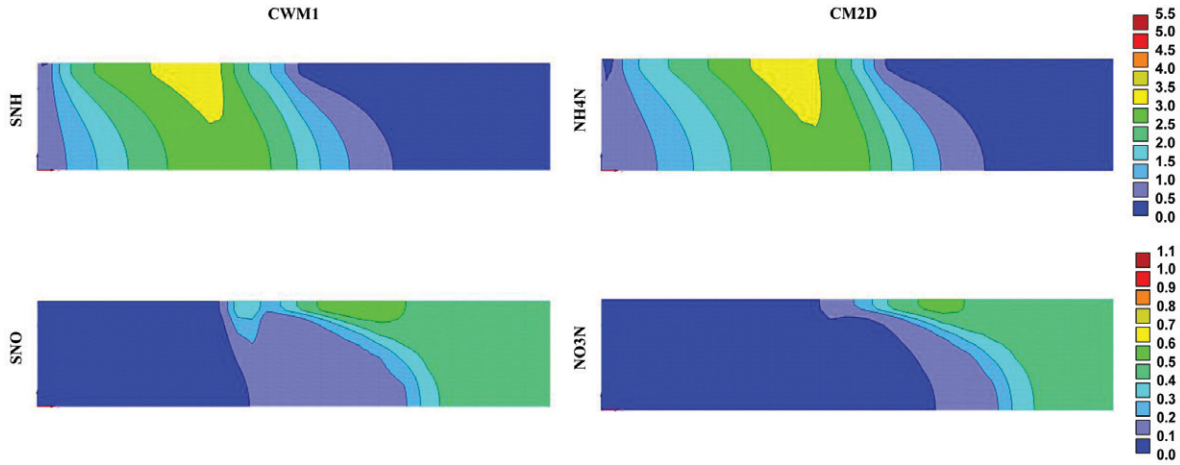

Fig. 7. Concentration profiles (mg L^{-1}) of NH_4– and NH_3–N (SNH4) (top left) and (NH4N) (top right), and NO_3– and NO_2–N (SNO) (bottom left) and NO_3–N (NO3N) (bottom right) simulated with HYDRUS using the CWM1 (left) and CW2D (right) biokinetic models.

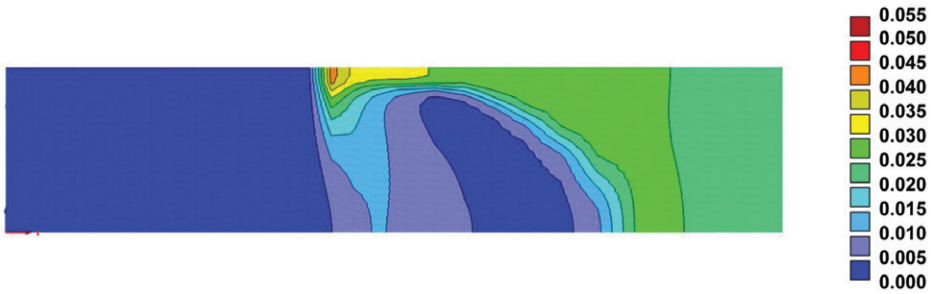

Fig. 8. Concentration profile (mg L^{-1}) of NO_2–N (NO2N) simulated with HYDRUS using the CW2D biokinetic model.

Fig. 9. Root water uptake distribution simulated with HYDRUS.

biomass was only found in the upper half of the HF bed. The same assumption—that the roots are dense in the upper 20 cm and then decrease rapidly with depth—was made here. In HYDRUS, solute uptake and release from roots is coupled to water flux. Because water uptake is assumed to be constant, O_2 release is constant as well. The root water and solute uptake parameters used are given in Table 6. The negative value of the cRoot variable for dissolved O_2 was used to model the O_2 release from the plant roots. The parameters in Table 6 resulted in a transpiration rate of 7.4 mm d^{-1} and a specific O_2 release of 5 g m^{-2} d^{-1}. The selected value of the specific O_2 release is a typical value reported for common reed [*Phragmites australis* (Cav.) Trin. ex Steud.], a plant species commonly used in CWs (Kadlec and Wallace, 2009).

Figure 10 shows how the O_2 concentration profiles are affected by the O_2 release. There is no dissolved O_2 available in the bed when the wetland plants are not considered (Fig. 10, top). Oxygen concentrations in the root zone when the O_2 release from plant roots is considered (Fig. 10, bottom) are also very low (0.01–0.02

Table 6. Root water and solute uptake parameters used in the example considering the influence of wetland plants.

Parameter	Value
Potential transpiration rate, cm d^{-1}	0.74
cRoot (NH_4), mg L^{-1}	50
cRoot (NO_3), mg L^{-1}	50
cRoot (dissolved O_2), mg L^{-1w}	−675

mg.L^{-1}). There is a constant supply of O_2 from the plant roots, however, that is readily consumed by aerobic microorganisms.

Figure 11 shows the bacteria concentration profiles of XH, XFB, and XA when the O_2 release from plant roots is either not considered (left) or considered (right). The bacteria concentration profiles of acetotrophic methanogenic (XAMB), acetotrophic SO_4–reducing (XASRB), and S^{2-}–oxidizing (XSOB) bacteria for conditions both with and without the O_2 release from plant roots are shown in Fig. 12.

Few aerobic bacteria are growing near the top of the water table when no O_2 is released from plant roots and is therefore available (XH and XA in the left part of Fig. 11 and XSOB in the left part of Fig. 12). The XFB bacteria are also growing only in regions where XH produces SF from hydrolysis. Other anaerobic bacteria, i.e., XAMB and XASRB, are growing in the rest of the filter bed, but their concentrations are rather low.

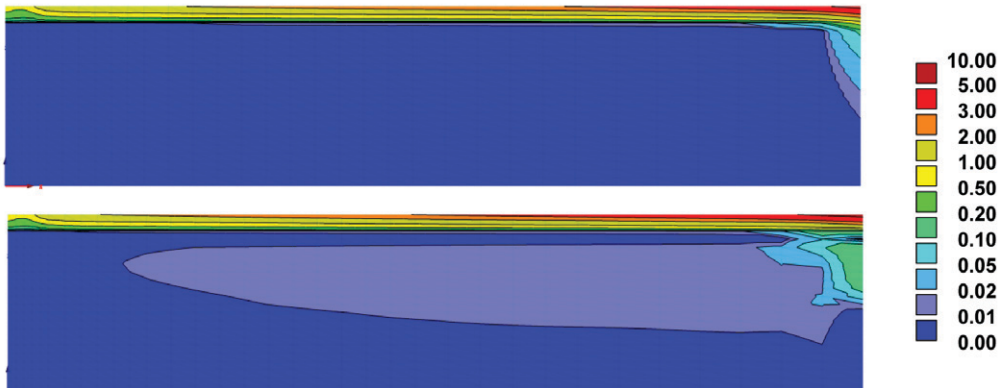

Fig. 10. Concentration profiles (mg L^{-1}) of dissolved O_2 (SO) simulated with HYDRUS using the CWM1 biokinetic model while not considering (top) and considering (bottom) the O_2 release by plant roots.

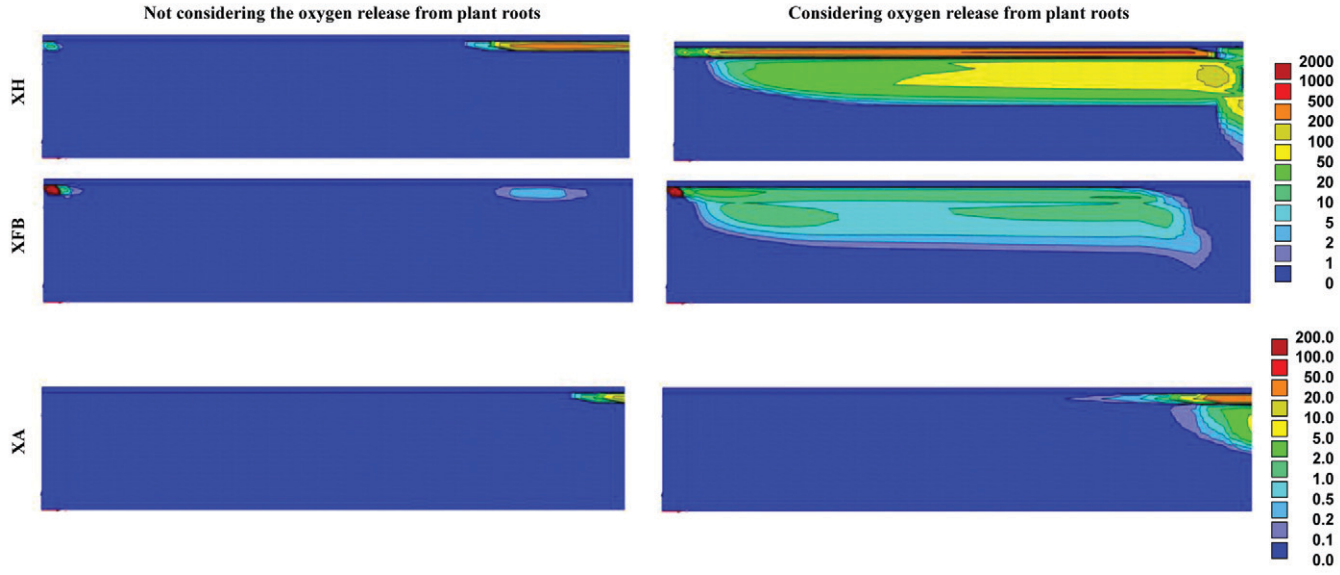

Fig. 11. Bacteria concentration profiles (mg kg^{-1}) of heterotrophic bacteria (XH) (top), fermenting bacteria (XFB) (middle), and autotrophic nitrifying bacteria (XA) (bottom) simulated with HYDRUS using the CWM1 biokinetic model while not considering (left) and considering (right) the O_2 release from plant roots.

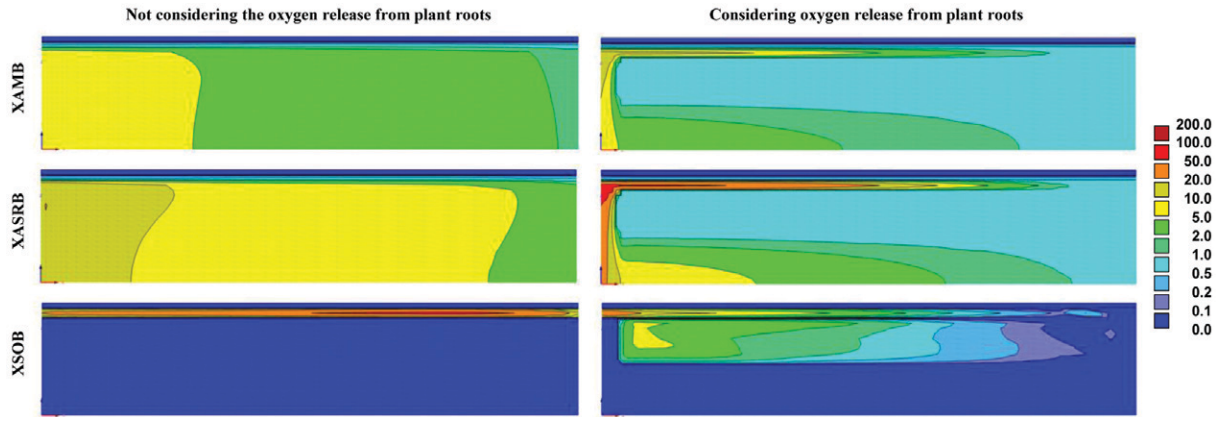

Fig. 12. Bacteria concentration profiles (mg kg^{-1}) of acetotrophic methanogenic bacteria (XAMB) (top), acetotrophic SO_4–reducing bacteria (XASRB) (middle), and S^{2-}–oxidizing bacteria (XSOB) (bottom) simulated with HYDRUS using the CWM1 biokinetic model while not considering (left) and considering (right) the O_2 release from plant roots.

When O_2 is released from plant roots (Fig. 11 and 12, right), the bacteria concentration profiles are completely different. The XH and XSOB bacteria are growing in the root zone. Due to the availability of SF, XFB can also grow in the root zone. Because the O_2 concentrations in the root zone are too low for autotrophic bacteria (XA), however, they can only grow at the end of the bed, where the organic matter has already been consumed (Fig. 11, right). Anaerobic processes occur only outside of the root zone, as indicated by the higher concentrations of XAMB and XASRB there (Fig. 12, right).

Table 7 compares the effluent concentrations simulated using CWM1 for conditions both with and without the O_2 release from plant roots. When using CWM1, the simulated COD effluent concentrations are similar for both conditions; however, the composition of the COD is quite different. When the wetland plants are not considered, the main part of COD is still biodegradable (XS), while when the wetland plants are considered, the main part of COD is inert (SI and XI). Effluent NH_3 concentrations are higher than in the influent, indicating that organic N was released as NH_3 during degradation of the organic matter and no nitrification occurred.

Table 8 compares the effluent concentrations simulated using CW2D for conditions with and without plants. There is a big difference in COD effluent concentrations whether the O_2 release from plant roots is considered or not. Without plants, the COD effluent concentrations are high, while with plants, they are comparable to the effluent concentration simulated using CWM1 (Table 7). Because CW2D does not consider anaerobic processes, degradation of the organic matter can only occur when O_2 from plant roots is provided. Llorens et al. (2011b) calculated that about 75% of the COD removal for this scenario was caused by anaerobic processes, thus clearly indicating the need to model anaerobic processes in HF CWs. Similarly to the CWM1 simulations, the effluent NH_3 concentrations are higher than in the influent, indicating the release of organic N and a lack of nitrification.

Table 7. Effluent concentrations simulated with HYDRUS using CWM1 for the example considering the influence of wetland plants. Chemical O_2 demand (COD) is shown in bold type. See Table 3 for parameter definitions.

Condition	SO_2	SF	SA	SI	XS	XI	COD	SNH_4	SNO
	mg O_2 L^{-1}							mg N L^{-1}	
Without O_2 release	<0.01	0.5	0.3	13.0	29.8	3.0	**46.6**	61.9	0.09
With O_2 release	<0.01	3.5	7.9	16.2	2.8	11.7	**42.1**	64.6	0.02

Table 8. Effluent concentrations simulated with HYDRUS using CW2D for the example considering the influence of wetland plants. Chemical O_2 demand (COD) is shown in bold type. See Table 3 for parameter definitions.

Condition	SO_2	CR	CS	CI	COD	NH_4–N	NO_2–N	NO_3–N
	mg O_2 L^{-1}					mg N L^{-1}		
Without O2 release	<0.01	84.7	27.8	30.2	**142.6**	60.5	< 0.01	< 0.01
With O2 release	0.01	0.2	2.5	42.9	**45.6**	71.7	0.01	1.95

Discussion

The CWM1 model (Langergraber et al., 2009b) has been proposed with the main goal of providing a widely accepted model formulation that would consider various biochemical transformation and degradation processes in CWs and that could be implemented in various simulation tools. Although CWM1 has been recently implemented into the RETRASO code by Llorens et al. (2011a, 2011b), Version 2 of the HYDRUS wetland model provides the first implementation of CWM1 that is commercially available.

The main difference between CWM1 implementations in RETRASO and HYDRUS is that RETRASO, contrary to HYDRUS, cannot consider a fixed biomass. Within a very simple example in Fig. 5, it was shown that bacteria concentration profiles that develop in HF beds are far more complicated than the constant profiles assumed by Llorens et al. (2011b). To maintain constant bacteria concentrations in the bed, Llorens et al. (2011b) had to add unrealistically high concentrations of bacteria to the influent water. The bacteria concentration profiles simulated using HYDRUS appear to be much more realistic than those simulated using RETRASO.

Version 2 of the HYDRUS wetland module (Langergraber and Šimůnek, 2011) includes two biokinetic models that have been developed to describe transformation and degradation processes in CWs treating wastewater. In addition to CWM1, the HYDRUS wetland module also includes CW2D (Langergraber and Šimůnek, 2005). The CW2D code was already implemented in the first version of the HYDRUS wetland module (Langergraber and Šimůnek, 2006). In contrast to CWM1, CW2D does not consider any anaerobic processes. The CW2D biokinetic model was originally developed to model VF CWs and only later was also applied to model HF beds. Reasonably good results were obtained with CW2D for low-loaded HF beds (e.g., Toscano et al., 2009). Table 9 provides guidance on which biokinetic model to use for different types of CWs and for what type of CW processes. As mentioned above, CW2D models nitrification as a two-step process and considers P, whereas CWM1 also includes anaerobic processes and considers processes affecting S.

Both biokinetic models included in the HYDRUS wetland module have been developed to model CWs treating municipal wastewater.

Table 9. Different applications of the biokinetic models CW2D (Langergraber and Šimůnek, 2005) and CWM1 (Langergraber et al., 2009b).

Biokinetic model	CW2D	CWM1
Type of constructed wetland	vertical flow low loaded horizontal flow beds	vertical and horizontal flow
Processes	modeling retention of P modeling nitrification as a two-step process	modeling anaerobic processes modeling transport and fate of S

A number of studies have been published that show that good simulation results can be achieved especially for VF CWs (e.g., Langergraber, 2003, 2007; Langergraber et al., 2007). In addition to applications involving CWs treating municipal wastewater, the HYDRUS wetland model has been also used to model

- CWs treating combined sewer overflow (Dittmer et al., 2005; Henrichs et al., 2007, 2009; Meyer et al., 2008);
- CWs treating effluents of a wastewater treatment plant for irrigation purposes (Toscano et al., 2009);
- runoff from agricultural sites and the effects of streamside management zones (Smethurst et al., 2011).

In addition to the HYDRUS wetland module that considers various biochemical transformation and degradation processes, the HYDRUS software provides most of the other important submodels needed to model a SSF CW, as defined by Langergraber et al. (2009b). By solving the Richards equation for water flow in porous media under variably saturated conditions, HYDRUS provides a suitable model for water flow. As discussed by Langergraber (2008), the calibration of the water flow module is of great importance and a necessary tool for subsequently achieving good results with reactive transport modeling. The HYDRUS code solves the convection–dispersion equations for both heat and solute transport. Transport equations for single components are linked by reaction terms that are calculated using the biokinetic models.

We have shown above that considering wetland plants, i.e., O_2 release from wetland plant roots, significantly influences the simulation results. With HYDRUS, it is also possible to simulate the plant nutrient uptake, which is coupled with the plant water uptake. Using this option, it is possible to model O_2 release from roots; however, HYDRUS is not able to model growth, decay, or decomposition of the wetland plants.

The only submodel that was mentioned by Langergraber et al. (2009b) and that is not available in HYDRUS is an option to simulate the transport and deposition of suspended particulate matter and its influence on the hydraulic conductivity. As clogging of SSF CWs is still one of the main, often-occurring, operational problems; the inclusion of such a model would allow prediction of the failure of SSF CWs due to clogging.

Summary and Conclusions

We have presented Version 2 of the HYDRUS wetland module, which includes two biokinetic models for simulating biochemical transformation and degradation processes in CWs. The CW2D and CWM1 biokinetic models describe different processes affecting different water constituents. As such, the two biokinetic models may be used for different types of CWs. We have shown that the implementation of CWM1 into HYDRUS is mathematically correct. Additionally, the HYDRUS wetland

module allows simulation of a fixed biomass in the filter bed, which is essential for simulating SSF CWs. Considering the influence of wetland plants resulted in different profiles of various bacteria groups in the bed of HF CWs.

The following conclusions can be drawn:

- Version 2 of the HYDRUS wetland module is the only publicly available implementation of the CWM1.
- It is essential for modeling SSF CWs that fixed bacteria can be simulated.
- Because CWM1 is able to describe anaerobic processes, it is more suitable for modeling HF CWs, whereas CW2D is more suitable for VF CWs.
- The influence of wetland plants on various biochemical transformation and degradation processes due to the release of O_2 by plant roots in a HF bed is significant and therefore has to be considered.
- More experience needs to be gained in the use of the CWM1 biokinetic model.

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