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Recent developments in numerical modelling of subsurface flow constructed wetlands

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ABSTRACT

Numerical modelling of subsurface flow constructed wetlands (CWs) gained increasing interest during the last years. The main objective of the modelling work is, on the one hand, to increase the insight in dynamics and functioning of the complex CW system by using mechanistic or process based models that describe transformation and degradation processes in detail. As these mechanistic models are complex and therefore rather difficult to use there is, on the other hand, a need for simplified models for CW design. The design models should be premium to the currently used design guidelines that are mainly based on rules of thumb or simple first-order decay models. This paper presents an overview of the current developments on modelling of subsurface flow CWs based on the modelling work and model developments presented at the WETPOL 2007 symposium. Three kinds of models have been presented: simple transport and first-order decay models, complex mechanistic models, and a simplified model that has been developed for design of CWs. The models are presented and selected results are shown and discussed in relation to the available literature.

1. Introduction

During the last years an increasing interest in numerical modelling of subsurface flow constructed wetlands (CWs) has been observed. CWs are engineered systems designed to optimize the treatment conditions found in natural environments; consequently, CWs are complex systems that are difficult to understand. A large number of physical, chemical, and biological processes are active in parallel and mutually influence each other. Therefore, for a long time CWs have been often considered as "black boxes" and only little effort has been made to understand the main processes leading to wastewater purification. For the same reason, almost all the available design guidelines are based on empirical rules of thumb, such as those using the specific surface area requirements (e.g. Brix and Johansen, 2004; ÖNORM B 2505, 2005;

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DWA-A 262, 2006) or simple first-order decay models (e.g. Kadlec and Knight, 1996; Rousseau et al., 2004). The main objective of numerical modelling is to obtain a better understanding of the processes governing the biological and chemical transformation and degradation processes occurring in CWs, thus providing insights into the "black box" Once reliable numerical models are developed and validated against experimental data, they can be used for evaluating and improving existing design criteria.

Two main types of CWs are distinguished: surface flow and subsurface flow CWs (e.g. Kadlec and Knight, 1996; Kadlec et al., 2000; Haberl et al., 2003). Surface flow (SF) CWs are densely vegetated systems with open water surfaces and typically have water depths of less than 0.4 m. In subsurface flow (SSF) CWs, no free water level is visible. SSF CWs are further subdivided into horizontal flow (HF) and vertical flow (VF) systems depending on the direction of water flow through the porous medium (sand or gravel). To prevent clogging of the porous filter material, the use of traditional SSF CWs is limited to mechanically pre-treated wastewater, having low content of particulate matter. Compared to SF systems, the contact area of water with bacteria and substrate is much larger, which decreases the area requirement of SSF CWs (Vymazal et al., 1998; Haberl et al., 2003) while increasing the removal efficiency of the system. This work focuses on model developments for SSF CWs. Langergraber (2008) reported that to date only few numerical models are available and able to describe treatment processes in SSF CWs. Most of the literature on "models" for CWs is relevant to HF CWs and refers to simple first-order decay models (e.g. Rousseau et al., 2004; Stein et al., 2006) or still describes the CWs as a "black box" (e.g. Pastor et al., 2003; Tomemko et al., 2007) thus providing only a limited understanding of the studied facility. The number of mechanistic or process based models is instead very limited. Such models can be further distinguished between models describing only the hydraulic behaviour and single-solute transport, models describing reactive transport in saturated conditions such as in HF CWs, and reactive transport models for variably-saturated conditions that have the highest complexity and that can be used for modelling VF CWs as well as HF CWs. In this paper we summarize different contributions presented at the WETPOL 2007 symposium relevant to SSF CW model development and validation. We try to show some of the most recent findings in this area, and identify some of the aspects where further research is needed. Three different kinds of models are presented in the subsequent discussion: simple transport and first-order decay models, complex mechanistic or process based models, and a simplified model that has been developed for design of CWs. After presenting the basis of the models, results of the modelling work are presented, summarized and discussed.

2. Model description

2.1. *Simple transport and first-order decay models*

The first class of models we present in this paper consists of analytical, closed-form equations. The derivation of all the models belonging to this class is based on the fundamental laws governing water flow and solute transport (such as the mass balance and the advection–dispersion equation). By defining appropriate boundary conditions and making additional assumptions on system geometry and behaviour, the governing equations are simplified and reduced to simple closed-form formulas. These models have the obvious advantage that no special mathematical or numerical treatment is required to solve the equations for the variable of interest. However, the important drawback is that the validity of the results is limited to situations where the underlying assumptions hold.

While different works pointed out that such models are generally not suitable to model reactive and degradation processes in wetlands (e.g. Kadlec, 2000, 2003), simplified models are often useful tools for evaluating water flow and transport of inert solutes. Several of such methods exist and are routinely applied by practitioners to estimate residence time, degree of mixing and hydrodynamic dispersivity. Among these methods, some of the best known are (i) the method of moments, (ii) the dispersed plug-flow (DPF), (iii) the tanks-in-series (TIS) model and (iiii) the detention time gamma distribution (DTGD). Details of each method, strength and limitations can be found in the literature (e.g. Kadlec and Knight, 1996; Levenspiel, 1999; Kadlec, 2003). However, we would like to point out that all the approaches listed assume that the flow field can be somehow simplified to one-dimensional behaviour, and the effects of dispersion, heterogeneity and dead zones are lumped together in the hydrodynamic dispersivity term. This may introduce a significant error in the computation e.g. of the effective residence time, which also can have tremendous impact on the estimation of the degradation efficiency (Kadlec and Knight, 1996). Recovery rate can be sometimes a useful indicator of the effectiveness of the applied model; however, this parameter alone does not ensure that modelling results are correct.

Sandoval-Cobo and Peña (submitted for publication), Giraldi et al. (in press) and Mena et al. (2007) evaluated the reliability of these methods on both horizontal and vertical flow conditions, and compared the results obtained using different approaches on the same data set. Moreover, Sandoval-Cobo and Peña (submitted for publication) in parallel with the tracer experiment measured COD concentration profiles across the length of their pilot-scale HF CW, and applied some simplified first-order degradation equations to fit their experimental data. The closed-form equations used by Sandoval-Cobo and Peña (submitted for publication) are the same as those used for non-reactive transport, with an additional sink term to account for degradation and transformation. Additionally, the modified k–C^* model was also tested (e.g. Kadlec and Knight, 1996; Persson et al., 1999).

2.2. *Mechanistic or process based models*

The multi-component reactive transport module CW2D (Langergraber, 2001; Langergraber and Šimůnek, 2005) was used by several authors (Korkusuz et al., 2007; Langergraber, 2007b; Mena et al., 2007; Toscano et al., in press). CW2D was developed to model transport and reactions of the main constituents of municipal wastewater in subsurface flow constructed wetlands and is able to describe the biochemical elimination and the transformation processes for organic matter, nitrogen and phosphorus. CW2D was incorporated into the HYDRUS variably-saturated water flow and solute transport program (Langergraber and Šimůnek, 2006; Šimůnek et al., 2006a,b). The HYDRUS program 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 non-linear non-equilibrium reactions between the solid and liquid phases (Šimůnek et al., 2006b). The CW2D module considers 12 components and 9 processes. The components include dissolved oxygen, organic matter (three fractions of different degradability, i.e. readily- and slowly-biodegradable, and inert), ammonium, nitrite, nitrate, and nitrogen gas, inorganic phosphorus, and heterotrophic and two species of autotrophic micro-organisms. Organic nitrogen and organic phosphorus are modelled as nutrient contents of the organic matter, i.e. they are calculated as a percentage of COD. The biochemical elimination and transformation processes are based on Monod-type expressions used to describe the process rates. All process rates and diffusion coefficients are temperature dependent. The processes considered are hydrolysis, mineralization of organic matter, nitrification (modelled as a two-step process), denitrification, and a lysis process (as the sum of all decay and loss processes) for the micro-organisms. CW2D assumes a constant concentration of micro-organisms (and other compounds) in each finite element. The thickness of the biofilm is not considered (Langergraber, 2001). The mathematical formulation of CW2D is based on the mathematical formulation of the Activated Sludge Models (ASMs, Henze et al., 2000).

Brovelli et al. (2007) implemented a set of biological and geochemical reactions into the three-dimensional numerical simulator PHWAT (Mao et al., 2006). PHWAT has been developed for reactive transport in porous media and consists of three different modules (flow, transport and biogeochemistry) coupled with an operator-splitting technique. The flow module is based on MODFLOW (MacDonald and Harbaugh, 1988), which uses a finite difference scheme to solve the saturated water flow equation within the domain. The transport module is based on MT3DMS (Zheng and Wang, 1999). Several numerical solvers are available, thus making the code robust and flexible. The biogeochemistry module is based on PHREEQC-2 (Parkhurst and Appelo, 1999), a general purpose model for aqueous geochemistry. PHREEQC is extremely powerful and flexible, thus making PHWAT potentially able to handle all the reactions of interest for CW modelling. The biogeochemical reaction network is similar to that of CW2D, based on the ASM structure (Henze et al., 2000). Kinetic oxidation of carbon sources, organic matter hydrolysis, nutrient transformations and assimilation (nitrogen and phosphorous primarily) are modelled via Monod-type kinetic equations. Oxygen dissolution is accounted for via a first-order mass-transfer equation. Temperature dependence is included via the Arrhenius equation (e.g. Langmuir, 1997). While the ASM model consists of kinetic equations only, full water chemistry and sediment–water interactions can be modelled with PHREEQC and thus PHWAT. This allows modelling of the pH variations that influence biodegradation kinetics (Kadlec and Knight, 1996), as well as redox and surface complexation reactions. An important advantage of PHWAT is that, thanks to its modular structure, it can be extended to account for the coupling between flow and transport, e.g., pore clogging due to suspended solid deposition or biomass growth. The model has been developed very recently, and the validation of PHWAT with experimental data is currently on-going. Some preliminary results have been presented (Brovelli et al., 2007), showing reasonably good agreement with experimental data. However, model calibration has been found extremely difficult, due to the strong non-linearities of the mathematical model.

FITOVERT (Giraldi et al., 2008) was developed specifically to simulate VF CWs and considers therefore only a one-dimensional flow from the top to the bottom of the system. The dynamic formulation of the model allows simulating the typical non-stationary behaviour of VF CWs. Boundary conditions are provided to simulate both variable inflows and ponding at the surface and free drainage, drainage with a pressure head and no drainage at the bottom of the system. The hydraulic flow for unsaturated condition is described by means of the Richards equation, while the constitutive relationships among pressure head, hydraulic conductivity and water content are described using the van Genuchten parameterization. Evaporation at the CW surface and transpiration through plants are also considered. FITOVERT describes biochemical processes of organic matter and nitrogen by means of the standard ASM (Henze et al., 2000). Advective and diffusive transport of contaminants in the liquid phase is implemented according to a mass conservation equation with a limited change to the dispersion term. Gas transport and transfer to the liquid phase are described for the oxygen by a mass balance with advection and dispersion. Settling and filtration of particulate matter is included thus allowing porosity reduction due e.g. to bacteria growth and to deposition of particulate components, so that the clogging process could be also simulated; the effect of pore size reduction on the saturated hydraulic conductivity is also considered. Giraldi et al. (in press) used the DPF model implemented in FITOVERT.

2.3. *Simplification of complex models*

Meyer et al. (2007) developed a simplified reaction model for CWs treating combined sewer overflow (CSO), also known as retention soil filters (RSFs), based on experiences with CW2D (Langergraber and Šimůnek, 2005). The background for this work was that the German design- and operation-guideline for RSFs (DWA-M 178, 2005) introduced the definition of the annual hydraulic load (in m^3/m^2) by calculating CSO volumes as result of long-term simulations of combined sewer-systems as a main criteria for filter design. Therefore the objective was the development of a tool that allows long-term simulations and can be combined with pollution-load-models for sewer-systems to optimize RSF design and operation.

Based on their experience Meyer et al. (2007) concluded that modelling of CSO treatment in CWs to optimize design and operation requires a reasonable balance between detailed description and practicable handling. The use of complex models like CW2D has been shown to be not practicable for long-term simulations in combination with sewer-system models (Dittmer et al., 2005; Meyer et al., 2006; Henrichs et al., 2007). Based on this experience and further experience from long-term simulations with KOSMO (Kaufmann and Schmitt, 2005) a RSF module for KOSMO has been developed. The module RSF_Sim (Retention Soil Filter Simulation) is not directly embedded into the KOSMO simulation program. RSF_Sim input data either can be generated manually using a graphical user-interface or can be imported directly from KOSMO.

RSF_Sim is able to describe filter layers whereby water flow is described using a sequence of stirred reactors with variable water contents (Fig. 1). At the beginning of loading events the retention layer (air) on top is filled as long as the loading rate is higher than the infiltration rate into the filter body. The RSF filter body consists of cover layer (gravel), filter layer (sand) and drainage layer (gravel). The infiltration rate into the RSF is determined by the hydraulic conductivity of the sand. The outflow of the drainage layer is limited to a maximum flow rate (lower than the hydraulic conductivity of the filter layer). In the case of very big rain events the rising water level in the system (dotted line) can lead to overflow. As a special feature the filter layer itself is divided into two layers thus allowing to describe different processes at different depths of the filter separately.

Meyer et al. (2007) assumed that all processes occur only in the sand layers, i.e. filter layers 1 and 2. Processes considered are:

"F" — Filtration: filtration of large particles on layer surface (filter layer 1) and of small particles in layer space (filter layer 1+2),
"S" — Sorption described by Freundlich-isotherms,
"D" — Degradation described by a decay rate.

Combinations of the processes are possible (e.g. "FD" and "SD"). Additionally, the process "SP" describes degradation of ammonium nitrogen only in dry periods between loadings (dry periods between loading events can be extensive, e.g. Uhl and Dittmer, 2005). Filter sand performance can be increased

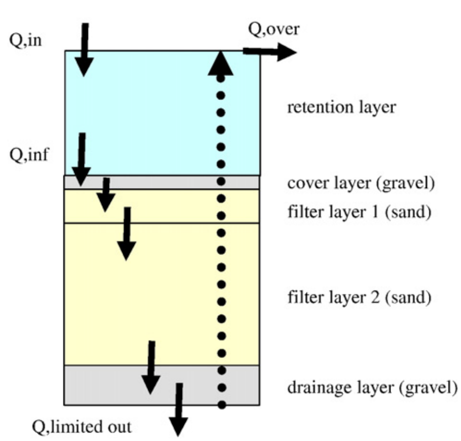


Fig. 1 – RSF_Sim hydraulics as a sequence of stirred reactors with variable water contents (Meyer et al., 2007).

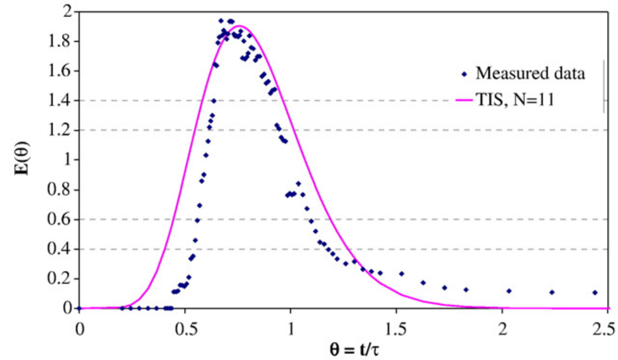


Fig. 2 – Characteristic TIS model fitting to tracer data (Sandoval-Cobo and Peña, submitted for publication).

or decreased for each pollutant separately, and all degradation processes are temperature dependent.

According to Meyer et al. (2007) first simulation runs with RSF_Sim gave plausible results. However, no calibration and validation of the model has been carried out up to now. As a next step Meyer et al. (2007) plan to calibrate the RSF_Sim module parameters for single events and long-term scenarios. Measured inflow- and outflow-curves shall be used for validation with manual data input before using RSF_Sim in combination with KOSMO as a design tool.

3. Results

3.1. *Simple flow and transport models*

3.1.1. *Modelling of HF CWs*

Sandoval-Cobo and Peña (submitted for publication) presented a study on HF CWs located in Columbia. The pilot-scale HF CW (9 m length, 3 m width and 0.6 m depth) received the effluent of an anaerobic pond treating domestic sewage and was planted with *Phragmites australis*. The unit was designed to receive a hydraulic loading rate (HLR) of 0.19 m d^{-1} of domestic wastewater with mean influent concentrations of 136 mg COD L^{-1}, 116 mg BOD_5 L^{-1}, 45 mg NH_4–N L^{-1} and 5 mg PO_4–P L^{-1}. Tracer experiments with an organic fluorescent tracer Rhodamine WT (RWT) were performed to describe the hydraulic behaviour of the system.

For wastewater characterisation samples were analyzed for COD, BOD_5, NH_4–N, NO_3–N, NO_2–N, PO_4–P, pH and temperature. In order to evaluate longitudinal COD concentration profiles and to obtain removal rate constants (*k*) across the wetland length, samples were taken from four sampling locations along the experimental unit centre line (at the influent, at 1/3 and 2/3 of the length, and at the effluent).

Six tracer experiments were conducted, and results were analyzed using three simplified models. One of the characteristic residence time distributions (RTDs) and the corresponding fitted curve for the TIS model is shown in Fig. 2. Basically, all six outflow tracer response curves produced skewed bell-shaped RTDs with long tails, as observed in previous tracer studies carried out on HF CWs (Chazarenc et al., 2003; Marsilli-Libelli and Checchi, 2005).

Table 1 – Hydraulic parameters for different models (SD = standard deviation).

Tracer run	t_0 (h)	Method of moments		DPF model	TIS model		
		τ(h)	R (%)	δ	N	τ_{TIS} (h)	R (%)
E1	35.6	41.3	N.A[a]	0.07	8	37.4	82
E2	35.6	42.9	61	0.05	11	39.6	73
E3	33.8	44.0	87	0.11	6	38.4	84
E4	33.9	49.2	91	0.11	6	41.2	91
E5	33.7	48.3	81	0.10	6	40.5	76
E6	33.5	53.9	75	0.16	4	43.3	75
Average	34.4	46.6	–	0.10	7	40.1	–
SD	1.0	4.7	–	0.04	2	2.1	–

[a] R = The whole mass recovery of tracer from each test (the value N.A accounts for unrealistic tracer recovery estimation due to instabilities experienced with the LIF meter used to determine Rd-WT concentrations in the first experiment).

Table 1 shows the hydraulic parameters calculated for each of the tracer experiments using different models: Method of moments, DPF and TIS models. The average real hydraulic residence times (HRTs) obtained were above the theoretical HRT value (t_0) for all models showing the inadequacy of hydraulic behaviour expected from the plug-flow based models. This can be explained by the fact that homogeneous velocity profiles ($\tau = t_0$) in HF CWs never occurs. Key factors such as porosity change due to biofilm accumulation, plant colonization and evapotranspiration (ET) rates must be taken into account. For example, plant density increased from 6 to 150 plants m^{-2} during the 5 months of experimental work while plant roots occupied the whole wetland depth. Average ET in the planted unit was calculated from water mass balance. Sandoval-Cobo and Peña (submitted for publication) found that about 29% of the water was lost due to ET, thus dramatically changing the hydrodynamics of the system. These two aspects must be considered when designing HF CWs under particular environmental conditions.

First-order degradation models (PF, modified k–C^*, DPF and TIS models) were fitted to data of COD concentrations versus the fractional distance (Table 2 and Fig. 3). The parameters describing the hydraulic behaviour, the dispersion number δ for the DPF model, and the number of tanks (N) for the TIS model have been taken from Table 1. Values for COD removal rate constants (Table 2) were obtained by applying each model to average COD concentration profiles measured. The optimization goal was firstly to fit the effluent concentration and secondly the concentration profile.

A good match to the experimental data could be obtained only for the k–C^* model. Plug-flow based models, i.e. PF, DPF and TIS models, k resulted in similar values when matching the effluent concentrations but did not fit the COD profiles measured. Sandoval-Cobo and Peña (submitted for publication) fitted all six measured concentration profiles separately and found the calibration of the k–C^* model parameters lead to obtaining a good correlation ($r^2 \geq 0.98$) for all six data sets. Moreover, the average values of the k and C^* parameters were between those reported for HF CWs (Rousseau et al., 2004).

Table 2 – Parameters for first-order decay models obtained for the data from Sandoval-Cobo and Peña (submitted for publication).

Model	k–C^*		PF	DPF	TIS
Parameter	k (d^{-1})	C^* (mg L^{-1})	k (d^{-1})	k (d^{-1})	k (d^{-1})
Value	4.21	55	0.88	0.90	0.96

Influent concentration C_0 = 136.5 mg COD L^{-1}.

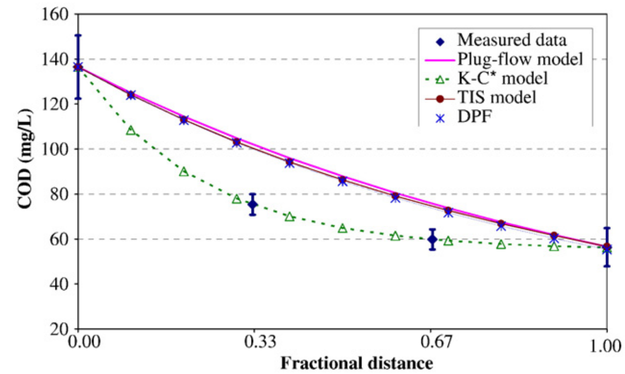


Fig. 3 – Comparison of measured (averages and standard deviation, n = 6) and modeled COD concentrations.

The values of k for CWs vary widely when compared to other wastewater treatment systems (Stein et al., 2006). The raw data series from which Table 2 mean figures were calculated show that k values for all models varied consistently throughout the six experiments. This feature has strong implications in the design of full-scale HF CW systems and reinforces the idea expressed by some authors about the convenience of using design parameters obtained from previously tested pilot units or HF CW operating under similar conditions (Rousseau et al., 2004). The combined use of dispersion studies and simplified mathematical models to evaluate the performance of organic matter removal in HF CW allowed obtaining more realistic key design parameters. The consideration of both flow dynamics and first-order kinetics leads to more sensible rate constant values that may have strong implications for the design and evaluation of HF CWs treatment units located in tropical regions.

The results obtained herein show that the k–C^* model reproduced well the performance of HF CWs in tropical regions, thus, the model may be used for design purposes provided that overall rate constants and characteristic hydraulic parameters are properly derived from experimental data.

3.1.2. *Modelling of VF CWs*

Giraldi et al. (in press) analyzed a VF bed that was part of a CW pilot plant operating as a tertiary treatment system after the Soreq Mechanical Biological Wastewater Treatment Plant serving the metropolitan area of Tel Aviv (Israel). The plant has been in operation since February 2005. The bed analyzed was a 33 m^2 VF CW with a total depth of 68 cm and 6 gravel layers (listed from the top to the bottom): (1st) 3 cm depth, particle size: 20–30 mm, (2nd) 9 cm depth, particle size: 2–3 mm, (3rd) 8 cm depth, particle size: 5–10 mm, (4th) 8 cm depth, particle size: 8 mm, (5th) 15 cm depth, particle size: 3–6 mm, (6th) 20 cm depth, particle size: 50–60 mm. The system was planted with

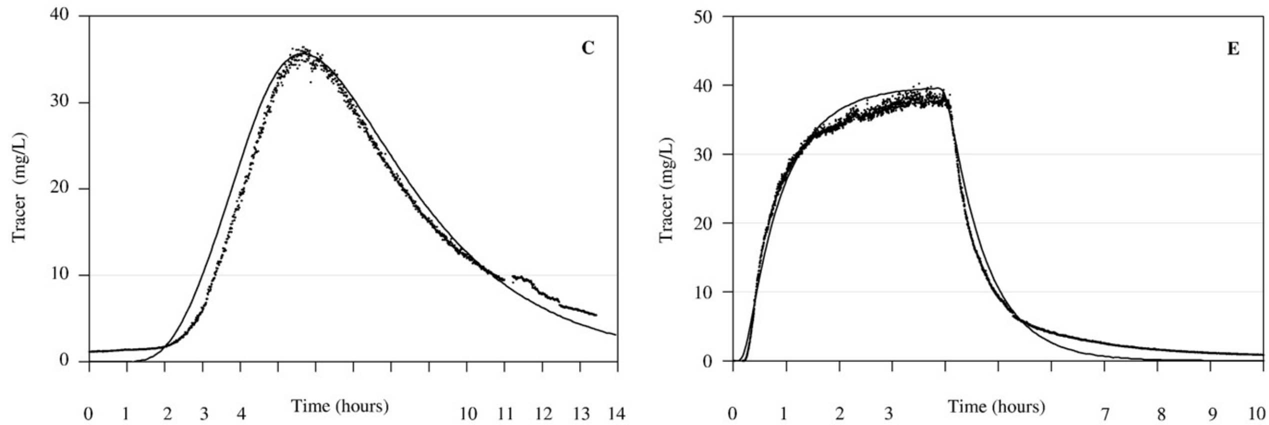


Fig. 4 – Experimental tracer breakthrough curves (dots) and numerical simulations (lines) for complete saturation (Test C, left) and free drainage (Test E, right); Giraldi et al. (in press).

different plant species: *Cyperus papyrus*, *Canna* sp., *Iris pseudoacorus*, *P. australis* and *Juncus ensifolius*.

Five tracer tests were performed with RWT for different hydraulic loads and saturation levels of the VF bed. The tracer tests were carried out in steady state conditions, feeding the system with controlled tap water flow and dosing RWT as square input signals. Each tracer test was temporally limited within a single workday for technical and safety reasons. No rain occurred during the tests.

Two experimental tracer breakthrough curves and the respective simulation results are reported in Fig. 4, while complete results of the RTD analysis are reported in Table 3, along with the main experimental parameters of the tracer tests. Background tracer concentrations were always negligible and the square input signals allowed obtaining well defined RTD curves within single workday intervals.

The mean residence time was always lower than the nominal retention time (when calculated), so the presence of dead zones in the bed could be highlighted. RTD analysis indicates that the HRT and the degree of apparent mixing (i.e. variance) increase as the water content in the system increases and as the water flow decreases. On the other hand the degree of local mixing (i.e. dimensionless variance) increases as the saturation degree of the bed decreases and slightly increases with the hydraulic load. The mono-dimensional plug-flow with dispersion model for unsaturated conditions resulted very satisfying in simulating all the tracer tests, both for saturated and unsaturated conditions. Giraldi et al. (in press) found that the dispersivity (λ) decreases as the saturation of the system increases, reflecting the behaviour of the dimensionless variance. The correlation between dispersivity and water content is discussed widely in literature dealing with the mechanisms of water and solute transport in the vadose zone. For a saturated system, λ is a function of the characteristics of the porous medium (Ogata, 1970). Straub and Lynch (1982) reported that λ describes the variation of fluid velocity from its average value and that λ increases with the effects of channelling and non-uniformity of the porous medium. Therefore Giraldi et al. (in press) assumed a dependence of λ on the degree of saturation of the system, since the water content affects the uniformity of the flow inside the porous medium. In fact, for unsaturated conditions local mixing due to different flow paths should increase, while saturation conditions provide more uniform flow paths, thus reducing local mixing. For their case study Giraldi et al. (in press) found the dependency between dispersivity and saturation degree to be linearly decreasing, but more data on different unsaturated conditions need to be analyzed to confirm this statement or to validate any other non-linear relationships. This is important for future research: numerical models describing the behaviour of VF CWs should implement this kind of dependency in order to obtain meaningful simulations for the transport (and consequently the fate) of solute compounds inside these kinds of systems. This is required to simulate both standard operation of VF CWs (periodic pulse loadings with draining conditions) and innovative operation schemes like the Tidal Flow mode (percolating with progressive saturation and sudden outflow).

Table 3 – Main experimental parameters and results of RTD analysis (Giraldi et al., in press).

Test	Saturation	Hydraulic load	Inlet tracer concentration	Dosing period	Monitoring period	Tracer mass recovery	Mean residence time	Dimensionless variance	Dispersivity (λ)
Label		L/min	μg/L	min	h	%	min	–	cm
A	Partial	24	56	180	8	88	128	0.38	10
B	Complete	48	22	122	6	58	113	0.24	4.5
C	Complete	24	110	169	14	59	341	0.18	4.5
D	Draining	24	57	98	6	63	52	0.60	14
E	Draining	24	56	230	10	67	51	0.53	14

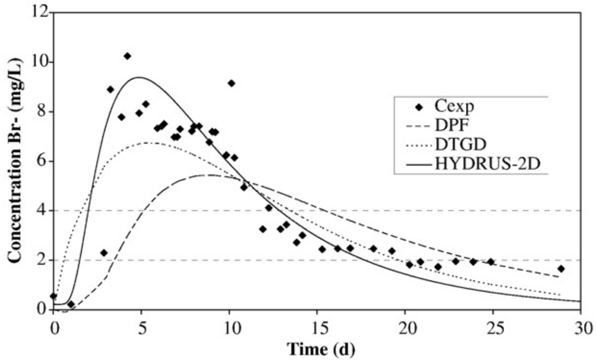


Fig. 5 – Comparison of experimental tracer concentrations to simulation results for CW1 (planted with *Phragmites australis*) using different models (according to Mena et al., 2007).

3.2. *Simulations with CW2D*

3.2.1. *Modelling of HF CWs*

Mena et al. (2007) presented simulation results of tracer experiments and multi-component reactive transport obtained for a pilot-scale experimental installation situated in southern Spain. The installation consisted of three parallel operated HF beds. Each bed consisted of a channel (size 2.5 m × 0.65 m with a depth of 0.6 m) with a longitudinal slope of 1%. Different species of macrophytes were planted: in CW1 *P. australis* (common reed), in CW2 *Lythrum salicaria* (purple loosestrife) whereas CW3 remained without plants. All beds were filled with gravel with a diameter of 6–9 mm (porosity 0.38), apart from the first and last 10 cm, for which the diameter was 9–12 mm (porosity 0.40) to improve the distribution of the wastewater in the inlet zone and to collect the treated wastewater in the outlet zone, respectively. The CWs were continuously fed with artificial urban wastewater. The mean influent concentrations have been 127 mg COD L^{-1} and 10 mg NH_4–N L^{-1} (Mena et al., 2007; Mena, 2008).

Tracer experiments were carried out using bromide. One litre solution of sodium bromide with a concentration of 5000 mg L^{-1} was fed by means of an impulse in each CW. So, the total tracer mass initially added was 5000 mg. After the pulse, wastewater feeding was kept running continuously and effluent samples were collected. Fig. 5 shows the experimental tracer concentration and the fit of the different hydraulic models for CW1. Mena et al. (2007) showed that for all experiments simulation with HYDRUS fitted better than DTGD and DPF models. Especially the DPF model did not fit very well to the experimental data mainly because the long skewed "tail" increases the mean HRT and this fact makes the DPF to be delayed in relation to the experimental data.

The experiments by Mena (2008) for pollutant removal have not been designed for modelling purposes. Thus, only the mean effluent concentrations of the different parallel beds could be modelled by introducing different oxygen release rates for the different plant species. Oxygen release rates caused by *P. australis* (CW1) and *L. salicaria* (CW2) have been found to be 2.06 and 5.92 g O_2 m^{-2} d^{-1}, respectively; oxygen transport by diffusion into CW3 amounted to 5.38 g O_2 m^{-2} d^{-1}. Differences between the efficiency of nutrient and organic matter removal have been found not only because of the presence of plants but also because of the plant species.

Mena et al. (2007) concluded that plant species influence both the hydraulics in and the removal efficiency of HF CWs. The hydraulic behaviour is influenced due to plant growth

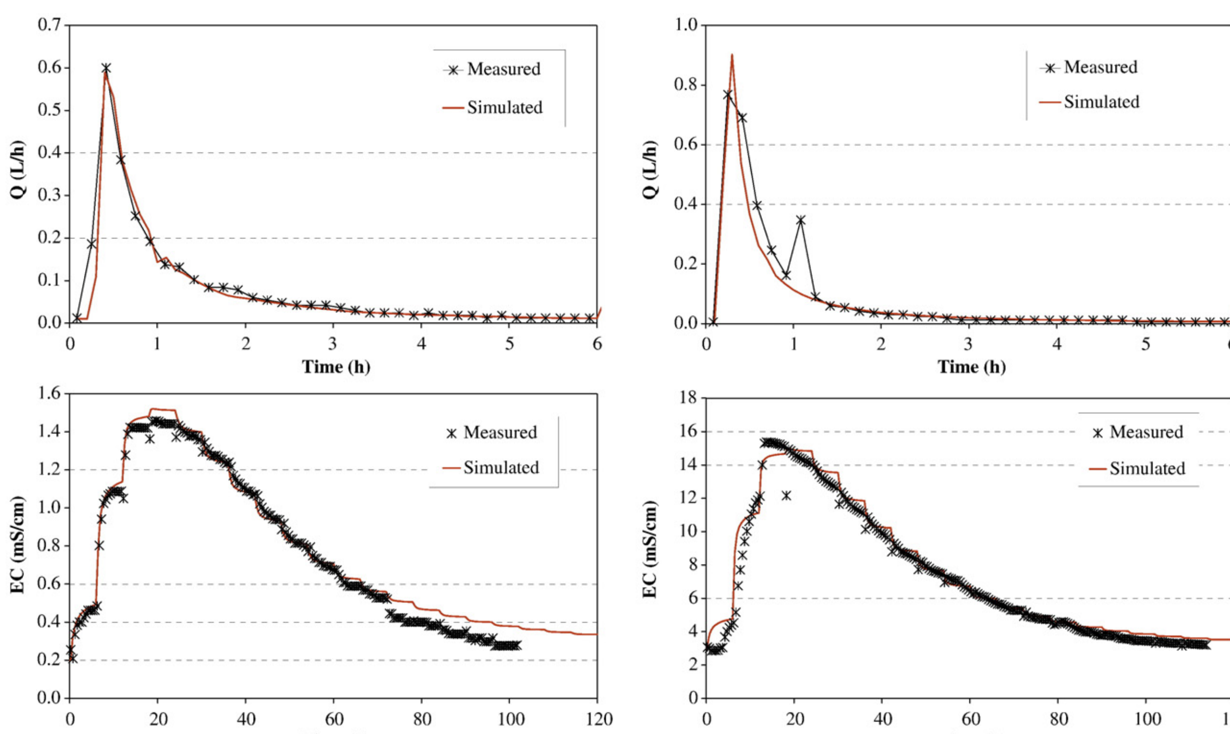


Fig. 6 – Simulated water flow (top) and tracer experiments (bottom) for Turkish (left) and Austrian (right) zeolite (Korkusuz et al., 2007).

increases ET and decreases dispersion, respectively. Tracer studies determined that the effective volume ratio can be higher than 1 caused by dead zones or hydraulic phenomena in which the tracer is accumulated and is being released gradually. The removal performance is influenced by plants as they can increase dissolved oxygen concentration and take-up nutrients but also because rhizospheric growth increases the surface area for biofilm development.

3.2.2. *Modelling of VF CWs*

Korkusuz et al. (2007) investigated 10 different natural and artificial substrates to be used for the main layer of VF CWs. Simulation results have been presented for lab-scale studies carried out at the technical lab of the Institute of Sanitary Engineering at BOKU (University of Natural Resources and Applied Life Sciences, Vienna). Each lab-scale column had a diameter of 20 cm and was filled with a 50 cm main layer using different substrates. The substrates (gravel size: 0–4 mm) tested were originally from Turkey (zeolite, sand, pumice, perlite, blast furnace granulated slag) and Austria (zeolite, sand, ferrosorp, crushed-concrete) and have been selected because they have a potential higher nitrogen and phosphorous adsorption capacity. The following parameters have been determined for all materials: particle and bulk density, porosity, saturated hydraulic conductivity and grain size distribution.

The lab-scale columns have been loaded four times a day with mechanically pre-treated municipal wastewater. Influent and effluent flow rates of 10 lab-scale columns have been measured. Tracer studies (with KCl dissolved in tap water) have been conducted to describe single-solute transport characteristics. Electrical conductivity of influents and effluents have been measured online and recorded with a data logger.

Fig. 6 shows simulation results for effluent flow rates from a single loading and from tracer experiments for two materials: Turkish and Austrian zeolite. The simulations have been carried out as follows: Measured values of bulk density, porosity and saturated hydraulic conductivity have been used as input parameters. Water flow has been calibrated using effluent flow rate measurements with the inverse simulation procedures implemented in HYDRUS (Šimůnek et al., 2006b). The parameters obtained for the flow model have been used for single-solute transport modelling of the tracer experiments. The simulations matched the measured data well for all columns. Korkusuz et al. (2007) pointed out that one main result of the study was the generation of input data sets for CW2D for different substrates. Further studies on reactive transport simulations regarding the removal efficiency are planned.

Langergraber (2007b) presented results from a simulation study using data from an experimental site located at the wastewater treatment plant Ernsthofen in Lower Austria (e.g. Langergraber, 2007a). A two-stage CW system that consists of two vertical flow beds with intermittent loading operated in series was investigated (Langergraber et al., in press). The first stage uses a grain size of 2–3.2 mm for the main layer and has a drainage layer that is impounded; the second stage a grain size of 0.06–4 mm and a drainage layer with free drainage. The two-stage system was operated with an organic load of 80 g COD m^{-2} d^{-1} for the first stage (1 m^2/person equivalent), i.e. 40 g COD m^{-2} d^{-1} for the whole system (2 m^2/person equivalent). The filter beds are planted with common reed (*P. australis*).

Langergraber et al. (in press) showed that the two-stage CW system performed better compared to a single-stage VF bed designed and operated according to the Austrian design standards (ÖNORM B 2505, 2005) with 4 m^2/person equivalent. The better performance resulted in lower effluent concentrations for low temperatures (below 6 °C) and an increased nitrogen removal of 53% at high average nitrogen elimination rates of about 1000 g N m^{-2} yr^{-1}, respectively.

Simulation results by Langergraber (2007b) showed that a more stable performance of two-stage CW system (compared to a single-stage VF bed) can be also predicted when the experimental plant is operated according to the testing procedures required for small wastewater treatment plants (ÖNORM EN 12556-3, 2001). Fig. 7 shows the simulated NH_4–N effluent concentrations of stage 1 and 2 of the two-stage CW system and of the single-stage CW system for an experiment with 2 days overload (2 days with 150% load within a 14 day period). The influent concentrations for the simulations have been 470 mg COD L^{-1} and 55 mg NH_4–N L^{-1}. The simulated NH_4–N effluent concentration of the two-stage CW system did not exceed 6 mg NH_4–N L^{-1} whereas effluent concentration of the single-stage VF bed exceeded 15 mg NH_4–N L^{-1} during the overload period. The results of these simulations still have to be verified with experiments at the experimental plant which are planned for 2008.

3.2.3. *Modelling of hybrid systems*

Toscano et al. (in press) presented simulation results for the hydraulic behaviour and effluent pollutant concentrations in a pilot-scale two-stage SSF CW for treatment of municipal wastewater. The experimental plant is located in San Michele di Ganzaria (Eastern Sicily). It was used for secondary or tertiary treatment and consists of four parallel lines each with two SSF beds in series. Each bed has a rectangular shape with a surface area of 4.5 m^2 (1.5 m × 3.0 m). For their study Toscano et al. (in press) used data from line 1 (planted with *Phragmite* sp.) and line 2 (unplanted), each comprising a HF and a VF bed in series. The HF beds were filled, to an average depth of 0.6 m, with volcanic gravel having a size of about 10–15 mm. The water depth in HF systems is about 0.55 m. The VF beds were filled with two different medium layers: volcanic sand as main layer for a depth

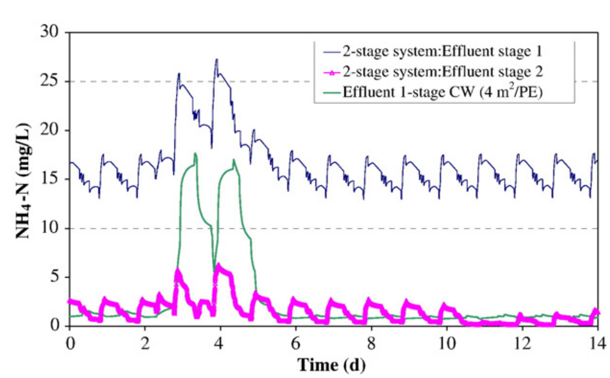


Fig. 7 – Simulated NH_4–N effluent concentrations for a period of 2 days overload.

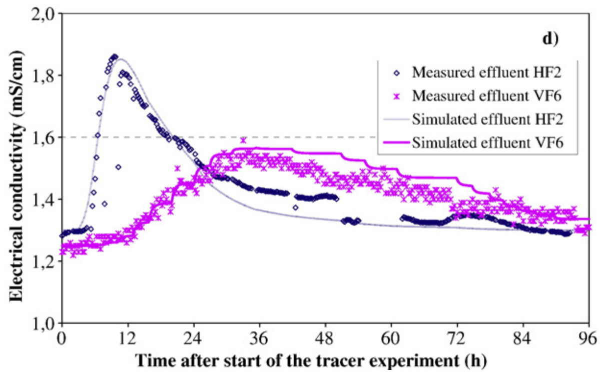


Fig. 8 – Measured and simulated data for a tracer experiment of line 2 (Toscano et al., in press).

of 0.5 m (about 0.06–4 mm; d_{10} = 0.13 mm; d_{60} = 2.0 mm) at the top of the filter bed and coarse volcanic gravel as drainage 472 layer (about 16–32 mm, 25 cm depth). The average influent flow rate for each line was about 40 ± 5 L h^{-1}.

Effluent flow rates measurements have been used to calibrate the flow model. Fig. 8 shows measured and simulated data for a tracer experiment of line 2 (unplanted). The simulated breakthrough curves matched the measured data well. For reactive transport the parameter set as proposed by Langergraber (2001) was used. Mean values for organic matter and nitrogen parameters could be simulated for both lines by considering nutrient uptake by plants and oxygen release by the plant roots. The influent concentrations for the simulations have been 23 mg COD L^{-1} and 22.1 mg NH_4–N L^{-1} for tertiary treatment and 64 mg COD L^{-1} and 8.6 mg NH_4–N L^{-1} for secondary treatment, respectively.

Since no significant changes of the influent concentrations over time occurred, a further experiment was conducted simulating influent ammonia variations and checking the answer of the model. This was done by adding ammonium chloride (NH_4Cl) as pulse tracer in the influent of lines 1 and 2 functioning as secondary treatment. In Fig. 9 measured and simulated NH_4–N concentrations are shown. The values for the parameters describing plant uptake and oxygen release obtained in the previous simulations have been used for the simulations. CW2D seems to be able to predict the dynamics in the effluent of the HF bed for both lines (Toscano et al., in press).

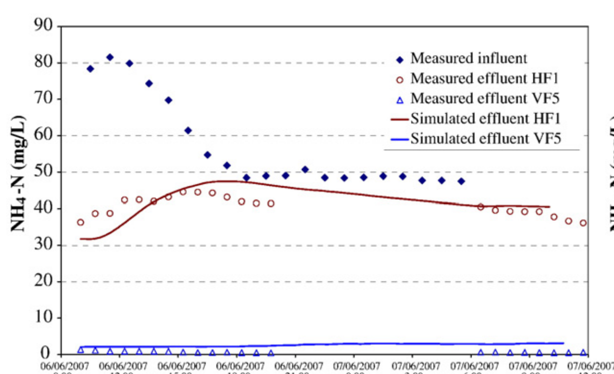
Toscano et al. (in press) concluded that the capability of HYDRUS/CW2D to model water flow and tracer experiments in both horizontal and vertical subsurface flow beds as well as to model the removal of some solute wastewater compounds was proved for hybrid systems.

4. Discussion

Most of the currently available literature aimed at modelling of CWs makes use of simplified equations. The underlying assumptions of such models are often that water flow can be considered homogeneous and mono-dimensional, or even simplified to plug-flow with or without hydrodynamic dispersion. Tracer experiments for HF CWs have been carried out by Sandoval-Cobo and Peña (submitted for publication) and Mena et al. (2007) and have been modelled using tanks-in-series (TIS), detention time gamma distribution (DTGD) and dispersed plug-flow (DPF) models. Mena et al. (2007) showed that for all their tracer experiments the simulations with HYDRUS (Šimůnek et al., 2006a) matched the data best and there was a poor match for DTGD and TIS models thus indicating that a mechanistic model such as HYDRUS also performs best for single-solute transport simulations in HF CWs.

Giraldi et al. (in press) found that mono-dimensional plug-flow with dispersion can be suitable to simulate both saturated and unsaturated conditions in VF CWs. The hydrodynamic analysis of Giraldi et al. (in press) also pointed out the correlation between dispersivity and water content for VF CWs; the dependency between dispersivity and saturation degree seems to be linearly decreasing. The same authors pointed out the need to introduce this dependency in the flow model for a successful modelling of VF CWs.

All hydraulic retention times obtained from experimental data have been found to be different than the calculated nominal retention times (Giraldi et al., in press; Sandoval-Cobo and Peña, submitted for publication; Mena et al., 2007). This can be explained because by the fact that homogeneous velocity profiles in HF CWs that are an underlying assumption of the simplified models never occur. Key factors such as the presence of dead zones, porosity change due to biofilm



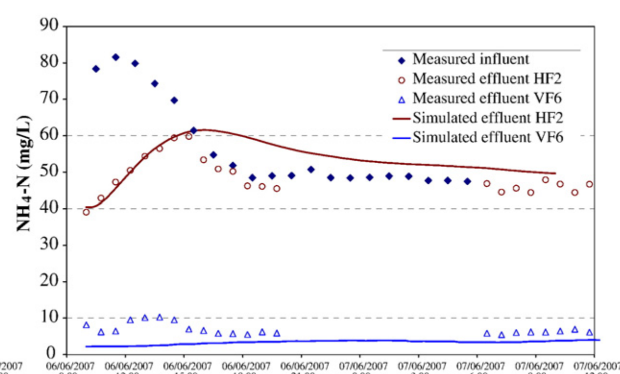


Fig. 9 – Measured influent concentrations and measured and simulated effluent concentrations of NH_4–N after the addition of NH_4Cl solution in lines 1 (left, planted) and 2 (right, unplanted) (Toscano et al., in press).

accumulation, plant colonization and evapotranspiration are not taken into account.

As for the biological cycling of nutrients and organic carbon, this models use simple first-order decay laws. Sandoval-Cobo and Peña (submitted for publication) tested some of these methods on HF CWs. For pollutant removal using first-order decay models Sandoval-Cobo and Peña (submitted for publication) concluded that k–C^* models reproduced well the performance of their HF CW and that k–C^* models may be used for design purposes provided that overall rate constants and characteristic hydraulic parameters are properly derived from experimental data. It has to be mentioned that the adequacy of the k–C^* model to describe pollutant removal in HF CWs may lay not on the typical background concentration interpretation but rather in the saturation-like kinetics shown by C^* value.

The k–C^* first-order degradation model is mostly applied to HF CWs to describe removal of organic matter (e.g. Rousseau et al., 2004; Mena, 2008). Other applications of the k–C^* model found in literature are e.g. batch fed systems for which Stein et al. (2006) estimated the temperature dependence of the model parameters of the k–C^* model for COD removal in a batch fed CW system for four plant species and Chan et al. (2008) modelled ammonia removal using the k–C^* model.

Different design models for HF CWs have been compared by Rousseau et al. (2004). By showing the output variability of these models it has been shown that the k–C^* model is the most suitable for design purposes. Already Kadlec (2000) concluded that first-order models are inadequate for the design of treatment wetlands. However, Rousseau et al. (2004) claimed that k–C^* model can be used for design only true when model parameters from systems operating under similar conditions (climatic conditions, wastewater composition, porous filter material and plant species) are available.

Langergraber (2008) reviewed mechanistic models available to simulate removal processes in SSF CWs. PHWAT (Brovelli et al., 2007) belongs to the category of models that can only describe saturated water flow and are therefore only applicable to HF CWs. This is due to the fact that the underlying model for water flow is MODFLOW which can only be used for saturated porous media. However, by using MODFLOW as a sub-model PHWAT uses the most advanced water flow model in this category as other models that are able to describe both carbon and nitrogen transformations under saturated water flow conditions use a tanks-in-series approach (Wynn and Liehr, 2001; Rousseau, 2005).

The model developed by Rousseau (2005) uses a reaction model that is presented in matrix notation based on the mathematical structure of the ASMs similar to the PHWAT reaction model structure. Rousseau's model describes aerobic, anoxic and anaerobic processes and has been applied to pilot-scale HF CWs to evaluate porosity decreases in experimental HF CWs submitted to different pretreatments (García et al., 2007).

Besides the multi-component reactive transport module CW2D (Langergraber, 2001) four models could be been found in literature that consider vadoze zone processes and are therefore suitable to simulate both HF and VF CWs. Langergraber (2008) reported that all these models are in a very early stage of development. Different approaches are used for modelling variably-saturated water flow, two models, Ojeda et al. (2006) and Wanko et al. (2006), using the Richards equation and therefore a mechanistic approach such as HYDRUS (Šimůnek et al., 2006a), whereas Freire et al. (2006) use a combination of CSTRs and dead zones and McGechan et al. (2005a) different layers through which water flows vertically trough the CW. CW2D is able to describe the biochemical transformation and degradation processes for organic matter, nitrogen and phosphorus in SSF CWs whereas Ojeda et al. (2006) describe processes affecting solids, organic matter, nitrogen and sulphur and Wanko et al. (2006) describe organic matter removal and oxygen transport only.

Recently a new mechanistic model (FITOVERT) was presented (Giraldi et al., 2008) that was developed to simulate VF CWs. The hydraulic sub-model of FITOVERT also uses the Richards equation to describe water flow in one-dimensional vertical layers. FITOVERT is able to simulate the fate of organic matter, nitrogen, particulates and oxygen transfer. First hydrodynamic simulations proved to be satisfying (Giraldi et al., in press) and the calibration of the biochemical parameters has already started.

Results using CW2D/HYDRUS (Langergraber and Šimůnek, 2005) showed that water flow, single-solute transport and reactive transport simulations resulted in good agreements with measured data for HF and VF CWs as well as for hybrid systems (Korkusuz et al., 2007; Mena et al., 2007; Toscano et al., in press). The practical applications have shown that simulation results match the measured data when the hydraulic behaviour of the system can be described well. A good match of experimental data to reactive transport simulations can then be obtained for CWs treating municipal wastewater using the values for the CW2D model parameters as given by Langergraber and Šimůnek (2005). Therefore it is advisable to measure at least the porosity and saturated hydraulic conductivity of the filter material to obtain reasonable simulation results for water flow (Langergraber, 2008).

For HF CWs the influence of plant species on the removal efficiency was shown by Mena et al. (2007) and Toscano et al. (in press). The removal performance has been influenced by plants as plants can increase dissolved oxygen concentration and take-up nutrients. Differences between the efficiency of nutrient and organic matter removal have been found not only because of the presence of plants (Toscano et al., in press) but also related to different plant species (Mena et al., 2007).

Meyer et al. (2007) used their experience from detailed simulations with CW2D (Dittmer et al., 2005; Meyer et al., 2006) to develop a simplified reaction model for CWs treating combined sewer overflow (CSO). The simplified reaction model models the hydraulics as a sequence of stirred reactors with variable water contents and considers only the most relevant processes (filtration, sorption and degradation). The differences between CWs for treating municipal wastewater and CSO have also been pointed out by Henrichs et al. (2007). They also used CW2D for simulating CWs for CSO treatment and found limitations such as that the degradation processes in dry periods should be different than those modelled in CW2D for organic matter degradation and nitrification. These limitations can be overcome by the RSF_Sim module as proposed by Meyer et al. (2007) that is planned to be used as a design tool.

To use mechanistic models to gain insights into complex systems such as "constructed wetlands" and to develop simplified design models based on these numerical simulations could be a way toward bringing more reliability into the design rules and to make modelling tools more acceptable for design purposes in practice. These simplified design models should comprise only the most relevant processes for the specific application and have therefore only few parameters. This can be of great importance for a better acceptance of models in the design of CWs. Even if a user-friendly operating environment is provided for mechanistic models making their use rather simple there are a lot of parameters to consider and it takes quite some time to gain experience with the using of these models.

5. Conclusion

Current developments in numerical modelling of CWs show two well-differentiated but related objectives. Firstly, mechanistic models aimed at gaining insight into wetlands dynamics and functioning, and secondly, simplified but robust and reliable models for design purposes. Both objectives need scientifically sound approaches and most likely the latter are a natural result of the former. Thus, joint work and proper communication between these two areas of research have to be pursued.

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This paper summarizes the findings on numerical modelling of subsurface flow CWs that have been presented during the 2nd International Symposium on "Wetland Pollutant Dynamics and Control WETPOL 2007" held from 16–20 September 2007 in Tartu, Estonia. The authors of the paper have been present and presented their work at WETPOL 2007 and especially thank their co-workers for their contributions.

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