Numerical modelling: a tool for better constructed wetland design?

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ABSTRACT

There is a need for a simplified computer-based design tool for subsurface flow constructed wetlands (CWs) which is based on process-based numerical models. Parameters of existing design guidelines and rules have been derived from experiments under specific conditions. Therefore designing CWs using these parameters is limited to these conditions (i.e. temperature, wastewater composition, filter material, etc.). Process-based numerical models describe the main processes in CWs in detail. If the design of CWs is based on these models it will be possible to design CWs for a variety of different boundary conditions and therefore the main limitation of existing design guidelines and rules could be overcome. The use of process-based models is currently limited mainly due to their complexity in structure and use. To make numerical modelling a useful and applicable tool for design, a simplified computer-based design tool that does not require special knowledge of numerical modelling is needed. Additionally, simple models for pre- and post-treatments are also required. Besides allowing designs for various boundary conditions, design tools based on process-based models can also predict the dynamic behaviour of the designed system thus showing e.g., the higher robustness of CWs against fluctuating inflows and peak loads compared to other treatment solutions. Such a tool could increase the quality of CW design and the acceptance and use of CW simulation in practice.

Key words | constructed wetland, design, process-based numerical model, simulation tool, subsurface flow

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INTRODUCTION

Constructed wetlands (CWs) are engineered water treatment systems that optimize the treatment processes found in natural environments. CWs are popular systems which efficiently treat different kinds of polluted water and are therefore sustainable environmentally friendly solutions. A large number of physical, chemical and biological processes are active in parallel and mutually influence each other (e.g. Kadlec & Wallace 2009). Therefore CWs are complex systems and for a long time have been often considered as 'black boxes'. Little effort has been made to understand the main processes leading to contaminant removal. Recently, some efforts have been made to understand the processes in CWs in more detail, and modern tools from environmental microbiology, plant biology, ecology and molecular biology have been used for this purpose (e.g. Faulwetter *et al.* 2009).

Because of the complexity of the processes in CWs, all the available design guidelines and rules are based on empirical rules of thumb, such as those using specific surface area requirements (e.g. Brix & Johansen 2004; DWA-A 262 2006; ÖNORM B 2505 2009) or simple first-order decay models (e.g. Rousseau *et al.* 2004; Kadlec & Wallace 2009). Rousseau *et al.* (2004) compared different design models for horizontal flow (HF) CWs whereby first-order degradation models have been shown to be the most suitable for design purposes. However, the authors claimed that accurate results can be obtained only when the parameters have been gained from systems operating under similar conditions (climatic conditions, wastewater composition, porous filter material, plant species, etc.).

During the last years an increasing interest in numerical modelling of subsurface flow (SSF) CWs can be observed. The main objective of numerical modelling of CWs is to obtain a better understanding of the processes governing the biological and chemical transformation and degradation processes, thus providing insights into the 'black box', and

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last but not least to evaluate and improve existing design criteria (Langergraber 2008). By using dynamic process-based numerical models, i.e., models that do not consider CWs as a 'black box' but describe main processes in detail, as the basis for design tools, it can be expected that the design tools will be more reliable and could be applied to a wide range of different boundary conditions.

In this paper the currently available process-based numerical models for subsurface flow CWs are presented briefly. The limitations of these models to be applicable as design tools are discussed and research questions are presented that need to be addressed on the way towards making process-based numerical models applicable for design purposes.

PROCESS-BASED NUMERICAL MODELS FOR CONSTRUCTED WETLANDS

During the last few years models with different complexities have been developed for describing processes in subsurface flow CWs. In subsurface flow CWs no free water level is visible, and water flows either horizontally or vertically through the porous filter media. Only a few models have been published that are able to model biochemical transformation and degradation processes.

HF systems can be simulated when only water flow saturated conditions are considered. A series or network of continuously-stirred tank reactors (CSTRs) is most frequently used to describe the hydraulics, and reactions are modelled with various complexities. For modelling vertical flow (VF) CWs with intermittent loading, transient variably-saturated flow models are 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 simplified approaches to describe variably-saturated flow.

The following list summarizes available process-based numerical models for subsurface flow CWs in which only models with minimum complexity in describing water flow and/or biochemical processes are listed. More information on the models can be found in recently published review papers (Langergraber 2008, 2010; and Langergraber *et al.* 2009a) and in the original references, respectively.

1. Complex flow models but single-solute transport only

- Schwager & Boller (1997): finite-element flow model, simulation of tracer experiments and oxygen transport in intermittent sand filters.
- Forquet *et al.* (2009): diphasic numerical model (based on finite-elements), description of the parallel movement of air and water in a VF filter.

2. Reactive transport models for saturated flow conditions

- Reactive transport models applicable only for constant flow rates:
  - Mashauri & Kayombo (2002): only carbon transformation processes.
  - Mayo & Bigambo (2005): only nitrogen transformations processes.
  - Wang *et al.* (2009): only nitrogen transformations processes.
- Reactive transport models with a tanks-in-series approach for water flow:
  - Chen *et al.* (1999): only carbon transformation processes.
  - Wynn & Liehr (2001): carbon and nitrogen transformation processes.
  - Marsili-Libelli & Checchi (2005): carbon and nitrogen transformation processes.
  - Rousseau (2005): carbon and nitrogen transformation processes, reaction model in matrix notation based on the mathematical formulation of the Activated Sludge Models (ASMs; Henze *et al.* 2000).
- Reactive transport models coupled to a complex groundwater flow model:
  - PHWAT (Brovelli *et al.* 2009a, b): carbon and nitrogen transformation processes, reaction model in matrix notation based on ASMs, coupled with the groundwater flow model MODFLOW, an extension of MODFLOW for unsaturated zones is on the way to being implemented.

3. Reactive transport models for variably-saturated flow

- Reactive transport models with simplified approached for simulating the variably-saturated water flow:
  - McGechan *et al.* (2005): different horizontal layers to describe variably-saturated water flow, considers pools of organic matter, ammonium, nitrate and oxygen; microbiologically controlled transformations between these pools.
  - FITOVERT (Giraldi *et al.* 2010): different horizontal layers to describe variably-saturated water flow,

reaction model in matrix notation based on ASMs for description of carbon and nitrogen transformation processes, implemented in Matlab®.
- ○ Freire *et al.* (2009): combination of CSTRs and dead-zones to describe variably-saturated flow, description of the removal processes for the dye AO7 only.

- Reactive transport models coupled with flow models that use the Richards equation to describe variably-saturated water flow:
  - ○ CW2D (Langergraber 2001; Langergraber & Šimůnek 2005): implemented in the HYDRUS software, reaction model in matrix notation based on ASMs for description of carbon, nitrogen and phosphorous transformation processes, has the most published applications.
  - ○ Ojeda *et al.* (2008): implemented in the RetrasoCodeBright (RCB) flow model, simplified description of organic matter, nitrogen and sulphur transformation processes.
  - ○ Wanko *et al.* (2006): considers organic matter removal and oxygen transport in VF filters.
  - ○ Maier *et al.* (2009): implemented in the MIN3P flow and transport code, describes processes in CWs for the remediation of contaminated groundwater.

The Constructed Wetland Model N °1 (CWM1), a general model to describe biochemical transformation and degradation processes for organic matter, nitrogen and sulphur in subsurface flow CWs, has been published with the main aim to provide a widely accepted model formulation for biochemical transformation and degradation processes in constructed wetlands that can then be implemented in various simulation tools (Langergraber *et al.* 2009b). CWM1 describes all relevant aerobic, anoxic and anaerobic biokinetic processes occurring in HF and VF CWs requiring predicting effluent concentrations of organic matter, nitrogen and sulphur. 17 processes and 16 components (8 solute and 8 particulate components) are considered.

FROM MODELLING TOWARDS DESIGN

Limitations of existing design guidelines and rules

Most of the existing design guidelines for CWs are based on empirical rules of thumb and/or simple first-order decay models. All these design models use parameters that have been derived from experiments with pilot CWs. Therefore the parameters are only valid for the specific boundary conditions for which they have been obtained i.e., under which the experiments have been carried out. These boundary conditions include: climatic conditions, wastewater composition, porous filter material, plant species, etc. For the design of a CW, this means that the parameters of these simplified design models can only be used for designing systems operating under similar conditions, such as climatic conditions, wastewater composition, porous filter material, plant species, etc. (Rousseau *et al.* 2004).

Experiences from applying existing simulation tools

A review of existing simulation tools for CWs showed that measured data from CWs can be matched (Langergraber *et al.* 2009a). Based on the experiences from the practical application of the HYDRUS/CW2D simulation tool Langergraber (2008) concluded that simulation results match the measured data when the hydraulic behaviour of the system is well described. The influence of the parameters of the hydraulic properties of the filter material is much higher compared to the influence of the parameters of the biokinetic model. Therefore once the flow model is calibrated well, a good match of experimental data to reactive transport simulations can be obtained using default parameter for the biokinetic model (such as given by Langergraber & Šimůnek 2005).

To obtain reasonable simulation results for water flow in VF beds, Langergraber (2008) advises to measure at least the porosity and saturated hydraulic conductivity of the filter material. For good fits of the flow model the measurement of the volumetric effluent flow rate between loadings is required. Additionally, tracer experiments should be carried out to get a better idea of the hydraulics and internal mixing.

Usually, the data obtained from CWs are based on grab samples that are collected from the influent and effluent on a daily, weekly or even only monthly basis. When using dynamic process-based models more frequent data are needed for calibration of the model to be able to utilize its full capacity, i.e., also to model and predict the changes in concentration over time. The number of additional samples needed for simulating CW depends on the objectives of the modelling study. Objectives of and the resulting efforts for modelling studies have been discussed in guidelines on the use of activated sludge models (e.g. Gillot *et al.* 2009). In the case that the variation of the influent concentrations is very low reactive tracers can be used to generate concentration changes. Toscano *et al.* (2009) showed the use of an ammonium peak as reactive tracer for a modelling study of two-stage experimental CWs.

Modern biotechnological tools can help to gain new insights into the functioning of CWs. However, data obtained from these experiments are usually not in a form and/or have the appropriate units to be used directly for modelling purposes. As an example, Langergraber *et al*. (2007) showed the conversion of measured data on the quantity of microbial biomass for modelling purposes. The measurements of Tietz *et al*. (2007) have been used as a starting point. They used several methods to measure microbial biomass including conversion from microscopic direct counts into biomass, fumigation-extraction for biomass-C, ATP measurements for biomass-C, and substrate induced respiration (SIR) for biomass-C (Figure 1, left). Langergraber *et al*. (2007) converted these data into microbial biomass COD which is the unit used in the simulation tools and showed that the simulation results matched the measured data well (Figure 1, right).

Another example is that the information gained from experiments and/or measurements can be of too much detail compared to the needs of the simulation tools and their underlying numerical methods. Figure 2 (left) shows a simplified picture of the reality in the subsurface:

- Between the sand grains there are pores filled with water, roots and (in the case of unsaturated conditions) air.
- The microbial biofilm is growing on the sand grains.
- Concentration gradients can be measured in the biofilm as well as in the pore water.

A number of simulation tools use the finite element method to numerically solve the governing partial differential equations for water flow and contaminant transport. Such a finite element is depicted in Figure 2 (right). A triangle is shown because most numerical methods use triangular shaped finite elements. In such a finite element it is assumed that there is a homogeneous distribution of sand grains, water and air, roots, biomass and contaminants. There is no distinction between the different phases in the finite element thus in every point in the finite element the same properties can be found, e.g., 55% sand, 30% water, 8% air, 4% roots and 3% microbial biomass. Information on biofilm thickness, concentration gradients, etc. is not available in a finite element. Data on e.g., biofilm thickness therefore can not be directly used for modelling but have to be converted into average biomass concentrations in the finite element. Gradients (of water content and/or biomass and contaminant concentrations) can only be found between different finite elements.

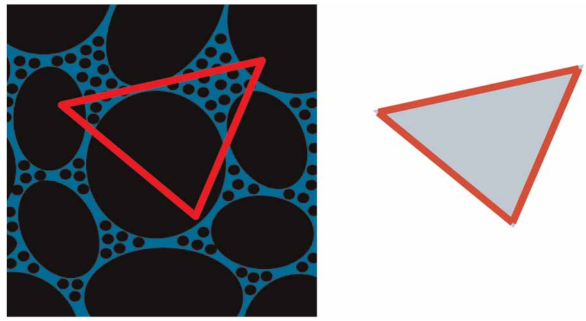

Figure 2 | Schematic sketch of the subsurface: the simplified 'reality' (left) and the finite-element approach (right).

Modellers have to communicate to specialists from other fields (e.g. microbiologists, plant physiologists, hydrologists, CW designers, etc.) which data are needed for modelling. However, these specialists also have to get a basic understanding of the input data requirements of the models. Only if a common language and understanding is found and joint efforts are made it is possible to design experiments and measurement campaigns in a way that useful data for modelling are produced.

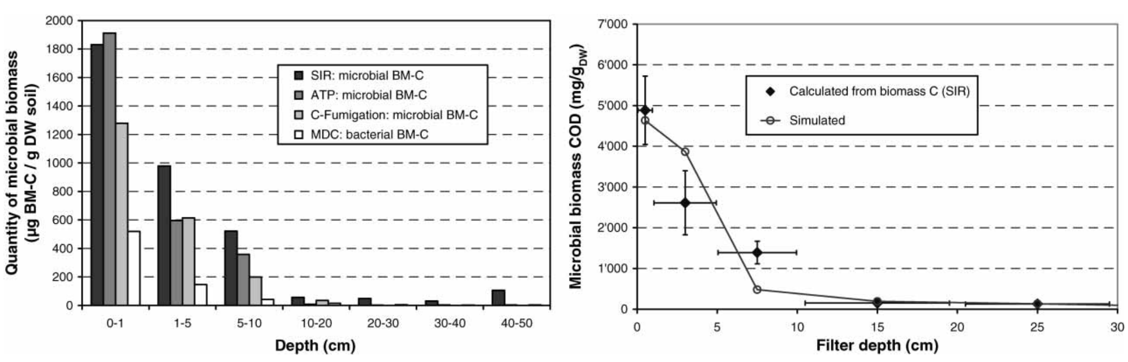

Figure 1 | Measured microbial biomass quantity (adapted from Tietz *et al*. 2007, left) and simulation results (adapted from Langergraber *et al*. 2007, right).

Limitations of existing simulation tools

Most of the papers on CW modelling published focus on the description of the biochemical transformation and degradation processes. However, a number of other processes have to be considered for the formulation of a full model for CWs (Langergraber *et al*. 2009b):

- The flow model (describing water flow in the porous media is of utmost importance).
- The influence of plants (growth, decay, decomposition, nutrient uptake, root oxygen release, etc.)
- The transport of particles/suspended matter and the description of clogging processes
- Adsorption and desorption processes
- Physical re-aeration

Even if simulation tools fulfil most of these requirements, there are two important aspects required for designing a CW, that none of the existing simulation tools has included yet. Two simple models for pre-and post treatment units would be needed:

1. a simple model for prediction of TSS and COD removal based on the design of the mechanical pre-treatment unit, and
2. a model for pre- and/or post-treatment of phosphorus with pre-precipitation in the mechanical pre-treatment unit and/or adsorption filters after the filter beds, respectively.

One of the main obstacles for the simulation tools available is that they are rather complicated and difficult to run. Although most of the tools have a graphical user-interface, it takes quite some time and experience to be able to produce realistic simulation results. Therefore only a few people in the organisations in which the tools have been developed are able to run them. Meyer *et al*. (2008) showed how, based on experiences from simulations with a complex simulation tool, a simplified but robust and reliable model for design purposes for CWs treating combined sewer overflow can be developed. This simple model has only a few parameters and is therefore simple to use.

The key factors influencing the treatment performance of CWs and their link to modelling

Microbial community

It is generally agreed that the microbial community plays a major role in the transformation processes and degradation processes in CWs. The resulting process conditions and the usually low flow rates in CWs lead to a high microbial diversity. Although there are a number of molecular-biological methods available to investigate these questions, knowledge of microbiological dynamics and the correlation of biological and non-biological processes in CWs is still insufficient (e.g. Faulwetter *et al*. 2009).

For modelling purposes the biomass characterization in subsurface flow CWs in terms of quantity and speciation is of utmost importance. In VF beds mainly aerobic processes occur and therefore mainly aerobic micro-organisms are present. Additionally, the number of heterotrophic micro-organisms is known to be much larger compared to the number of autotrophic micro-organisms (Langergraber *et al*. 2007). The situation is much more complicated in HF CWs where mainly anaerobic processes occur thus also requiring the consideration of sulphur transformation and degradation processes. At the moment there have been no investigations of the distribution of the microbial biomass and the actual concentrations of the specific bacteria groups that have been defined in biokinetic models, e.g., in CWM1 besides heterotrophic and autotrophic nitrifying bacteria, 4 other bacteria groups are also defined: fermenting, acetotrophic methanogenic, acetotrophic sulphate reducing and sulphide oxidising bacteria (Langergraber *et al*. 2009b). Thus information on the quantity and the distribution for all bacteria groups in the filter is required to be able to model realistic biomass distributions in the VF and HF beds.

To describe the kinetic rates of the biokinetic processes a determination of bacterial activities and rate constants is required. Respirometric tests are a promising tool, such as the advanced CW respirometry technology prototyped by (Andreottola *et al*. (2007), Figure 3) and further developed by Ortigara *et al*. (2010) and Morvannou *et al*. (2010).

Vegetation

Several major functions have been attributed to plants in SSF CWs, including physical filtering by root-mats, provision of surface area for attached microbes growth, insulation by aerial tissue and litter during winter, uptake and storage of nutrients and other elements, release of oxygen and other substances by the roots, and the contribution of organic carbon to the substrate (Brix 1997).

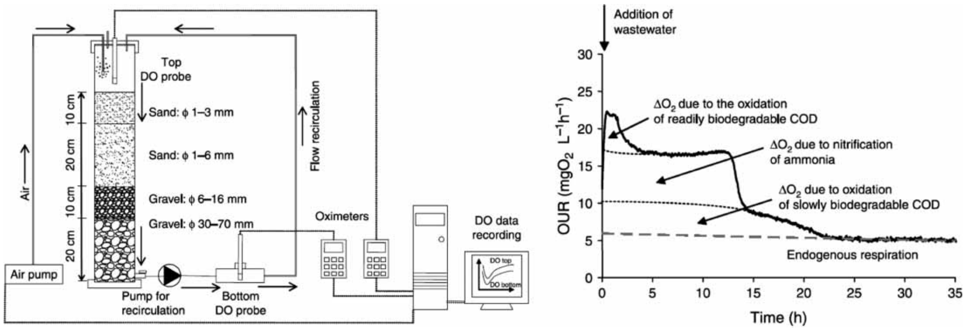

Figure 3 | Respirometer for monitoring oxygen consumption (left) and examples for a respirogramm (right) (Andreottola *et al*. 2007).

Plants are therefore an indispensable part of subsurface flow CWs. Therefore especially the following processes associated with plants are important:

- the water balance and the influence of plants on the hydraulics (e.g. evapotranspiration),
- the oxygen release and organic carbon release through the plant roots which influence the microbial processes in the subsurface, as well as
- the nutrient cycling (uptake and release of nitrogen and phosphorus) which influences the overall treatment performance.

Physical and other processes

The physical and physicochemical characteristics of the filter material used in a CW can greatly influence the overall performance of the system. Physical properties (such as porosity, hydraulic conductivity and grain size distribution) influence hydraulic efficiency, which is a critical component of good design. Poor hydraulic efficiency leads to short-circuiting and reduced treatment performance (Kadlec & Wallace 2009). The importance of the description of water flow for modelling defines the need to know the physical properties of the filter material (Langergraber 2008).

Additionally, the following physical and other processes are important:

- the physicochemical properties of the filter material are important to model e.g., adsorption,
- the hydraulic retention time in CWs that is an important factor for their treatment efficiency,
- the oxygen transfer, as oxygen is one of the most important environmental conditions for biokinetic processes, and
- the processes influencing clogging of the filter media and therefore changing the hydraulics and further influencing the performance of the CW.

SUMMARY AND CONCLUSIONS

Process-based numerical models for CWs have gained increasing attention in the last couple of years. As well as aiming to increase understanding of the system, models aim to improve existing design criteria for CWs. All the existing design guidelines and rules are based on empirical rules of thumb and/or simple first-order decay models and use parameters that have been derived from experiments. Therefore if the parameters derived from these experiments are used for design they are only valid for the specific experimental boundary conditions, e.g., climatic conditions, wastewater composition, porous filter material, plant species. It can be expected that when dynamic process-based numerical models are used as the basis for design tools, that the design tools can be applied to a wide range of boundary conditions and the limitations of existing design guidelines and rules can be overcome.

Can existing simulation tools for CWs now be used for the design of CWs? Existing simulation tools are able to describe the processes in SSF CWs in detail. However, development is still needed in terms of a better characterisation of the microbial biomass to be able to model realistic biomass distributions in HF and VF beds. Additionally, there are two main limitations of existing simulation tools being applicable as a design tool:

1. Although the simulation tools have graphical user-interfaces, they are complicated to use and it takes time and experience to be able to produce realistic simulation results.
2. Models for pre- and post-treatments are not available in the existing simulation tools but are required to carry out a design of a CW.

Therefore, to make numerical simulation a useful and applicable tool for CW design it can be concluded that a further development of the existing models is needed. A simplified computer-based CW design tool based on process-based numerical models should be developed that:

- can be used with knowledge of CW design but does not require special knowledge of numerical modelling,
- allows designing CWs for different boundary conditions (such as climatic conditions, wastewater characterization, filter material, climates, etc.), and
- makes the description of the dynamic behaviour of the designed CW possible thus allowing the demonstration of the greater robustness of CW treatment systems e.g., against fluctuating inflows and peak loads.

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