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NUMERICAL SIMULATION OF FLOW AND BIOKINETIC PROCESSES IN SUBSURFACE FLOW CONSTRUCTED WETLANDS: A SYSTEMATIC REVIEW

Malva A. Mancuso[1*] and Mariele Fioreze[2]

[1]*Department of Engineering and Environmental Technology, Federal University of Santa Maria, Brazil*
[2]*Department of Sanitary and Environmental Engineering, Federal University of Santa Maria, Brazil*

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Abstract: Constructed wetlands are engineered systems designed and constructed to treat wastewater using natural functions of vegetation, soils and microbial assemblages. Seeking the optimization of these systems, numerical simulation models have been developed in order to obtain parameters for design, representation of treating conditions and prediction of future scenarios. This paper reviews the state of the art on the numerical models for simulating flow and biokinetic processes in subsurface flow constructed wetlands. In this review, it is highlighted the application and performance of five software applied to simulate saturated horizontal flow (CWM1-RETRASO and PHWAT), variably saturated vertical flow (FITOVERT and HYDRUS-CW2D) and variably saturated vertical or horizontal flow (HYDRUS-CWM1). For vertical flow, FITOVERT requires less data input, but HYDRUS-CW2D simulates transformation of phosphorus and ammonia adsorption. For horizontal flow, HYDRUS-CWM1 and CWM1-RETRASO have similar approach in terms of species and number of reactions, but HYDRUS-CWM1 simulates the effect of transpiration and the limitations of bacterial growth. To simulate phosphorus in horizontal flow, the only applicable software is PHWAT, besides be able to simulate of gas production. In Brazil, a few studies address the subject of constructed wetlands simulation. Some of them apply software such as AQUASIM and MATLAB to support flow and transport equations.

Keywords: Biokinetic reactions; flow simulation; reactive transport; wastewater treatment

* Correspondence to: Malva A. Mancuso, Tel.: +55 55 374 40600 Ext 0643. E-mail: malvamancuso@ufsm.br

INTRODUCTION

Constructed wetlands (CWs) are artificial systems constructed in controlled operating conditions, in order to simulate biogeochemical cycles as observed in natural environments. Therefore, processes including vegetation, substrate (porous media) and microorganisms association assist in the wastewater treatment. The basic principle of these systems are the formation of biofilm attached to the porous media and the roots of plants, and the action of aerobic and anaerobic microorganisms, enabling the degradation of organic matter and the conversion of nitrogen by nitrification and denitrification processes (Platzer, 1999; Vymazal, 2000).

The CWs have been classified for a long time according to the hydraulic system into two groups: surface flow (SF-CWs) and subsurface flow (SSF-CWs) systems and, according to the flow direction, in horizontal subsurface flow constructed wetlands (HSSF- CWs) and vertical subsurface flow constructed wetlands (VSSF-CWs). Recently, a new approach was proposed, based not only on the hydraulic properties of the porous media (flow direction and saturation), but also in vegetative characteristics, being highlighted (Fonder & Headley, 2013) (**Fig. 1**):

(a) Surface flow constructed wetlands, horizontal flow, dominated by emergent herbaceous macrophytes (*SF*); (b) Surface flow constructed wetlands, horizontal flow, containing free-floating vascular aquatic plants growing on the water surface (*FFM*); (c) Surface flow constructed wetlands, horizontal flow, with emergent macrophytes growing on a buoyant structure (*FEM*); (d) Subsurface flow constructed wetlands, vertical flow, in which the flow direction is mixed, often periodically alternating between up and down flow (*FaD*); (e) Subsurface flow constructed wetlands, vertical flow, with free-draining substrate and subsurface loading (without surface flooding) (*VDF*); (f) Subsurface flow constructed wetlands, vertical flow, with a flooded surface for outflow (*VUP*), and; (g) Subsurface flow constructed wetlands, horizontal flow, with subsurface loading (without intentional surface flooding) (*HSSF*).

The first research evidences with CWs are dated from the 1950s and were developed by biologist Dr. Kathe Seidel at the Max Planck Institute, in Germany (Kadlec & Knight, 1996). Dr. Seidel used vertical filters to treat domestic wastewater, phenol-contaminated wastewater and agricultural wastewater. Later, in the 1970s, Reinhold Kickuth developed the Root Zone Method concept, to reference horizontal flow systems in porous media, used to allow the development of macrophytes and the biological activities (Verhoeven *et al.,* 2006). In Brazil, the first attempt to use the CWs systems was in the 1980s, when Salati and Rodrigues constructed an artificial lake near by a highly polluted stream in Piracicaba (São Paulo) (Salati *et al.,* 1999).

In the last 21 years, a third of the world's countries have made use CWs for wastewater treatment, being mainly countries in Europe, North America, Far East and Oceania (Zhi & Ji, 2012). Moreover, it is highlighted that the research related to this kind of treatment in developing countries are still incipient (Zhang *et al.,* 2014).

Experiments involving CWs in Brazil began to be published in the 1990s. The first studies used this technology to treat wastewater from rural areas (Conte *et al.,* 1992), pointed out the benefits of using the macrophyte *Typha* sp. in the treatment of domestic wastewater (Amorim *et al.,* 1997) and showing efficiency in the treatment of effluents after the septic tank (Philippi *et al.,* 1999). The studies about CWs have been intensified in the 2000s, with several arrangements regarding the shape, the layout of the constructed project and the system operation (Sezerino *et al.,* 2015).

The acknowledgement of the relevant factors involved in the treatment of effluents by CWs allows assessing the performance of each system. However, traditional studies on the CWs focuses on the efficiency of contaminants removal look at systems as a "black- boxes" from empirical approaches and do not distinguish between the different active removals processes (e.g., Pastor *et al.,* 2003, Tomenko *et al*., 2007). In addition, the non-uniformity of the projects design and the operational system leads to gaps and differences results on the treatment process. Despite the large number of investigations, design and optimization of the CWs are still based, mainly, on empirical equations, which results in an incomplete understanding of the functioning of the systems that sometimes can hinder the performance of the treatment processes about the functionality of the system performance.

In Brazil, there are no standards regarding to the CWs systems, which difficult the uniformity of the parameters and criteria for the design and operation. In the case of HSSF-CWs, the international literature is focused on the removal process of organic matter, and considers the system as a biological reactor of attached biomass with a first-order kinetic removal (Hammer, 1989; Conley *et al.,* 1991; Crites, 1994; Cooper *et al.,* 1996). In the case of VSSF-CWs, the models and the empirical criteria are focused on the balance of oxygen needed for the cleaning activities of organic matter and transformation of nitrogen series (Johansen & Brix, 1996; Platzer, 1999).

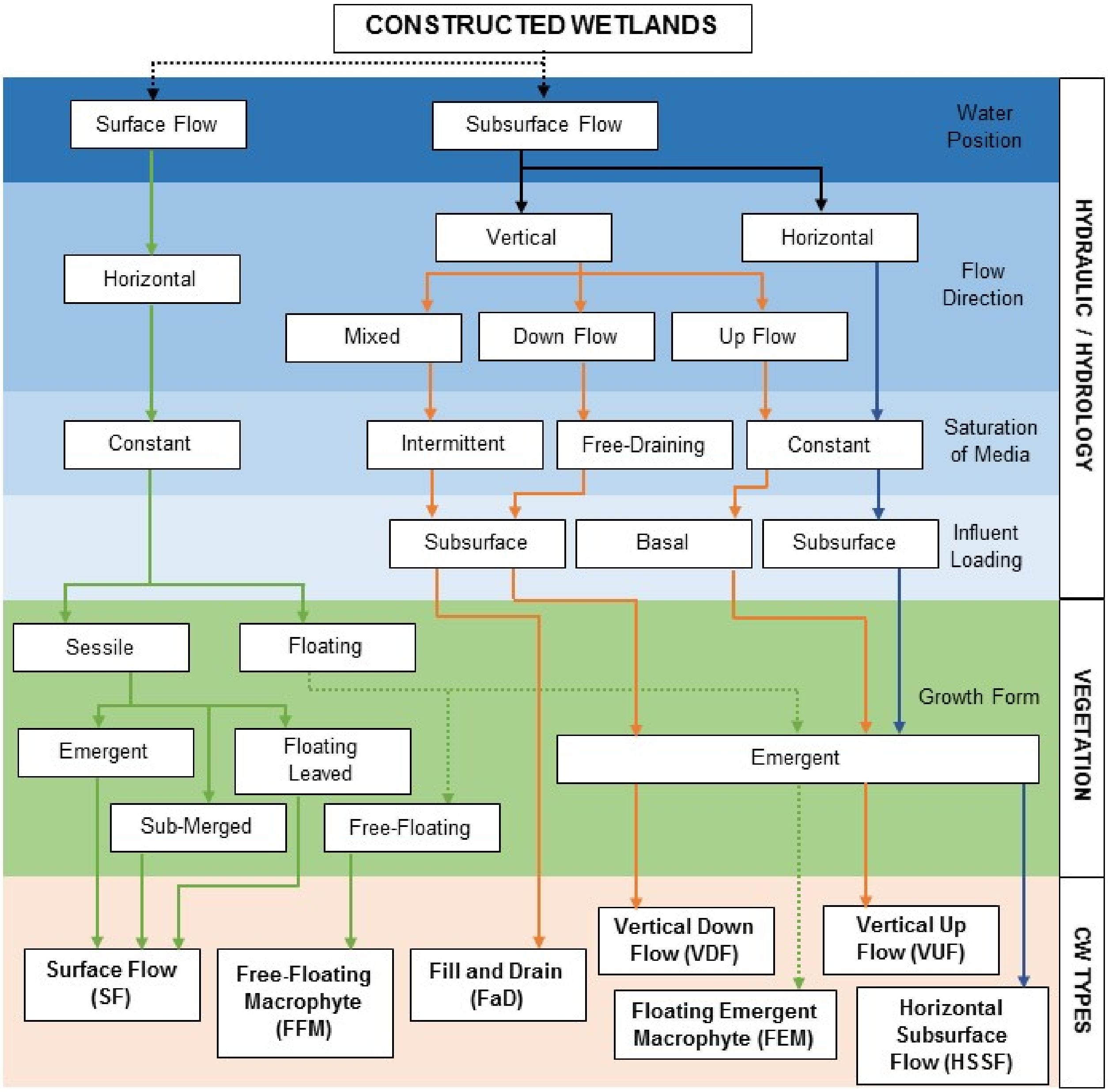

Fig. 1 Classification of constructed wetlands for wastewater treatment. Adapted: Fonder & Headley (2013)

The design of the CWs is also made base on the estimation of the required area according to the demand per capita. Data from the literature suggest a range of 0.5 to 3.0 m² per capita, to calculate the needed area for treatment of domestic wastewater with HSSF-CWs (Shrestha *et al.,* 2001). In the case of VSSF-CWs is recommended 1 m² per capita for BOD removal or 2.0 m² per capita to improve nitrification process (Cooper *et al.,* 1996). The Brazilian experience with HSSF-CWs, used to treat domestic wastewater shows that this relationship can range between 0.14 m² per capita (Avelar *et al.,* 2009) and 8.0 m² per capita (Borges *et al.,* 2008).

A simplified computer-based design tool for subsurface flow constructed wetlands simulation, allowed to improve the CWs processes, by testing parameters as the inflow of the system, the size and geometry design, the particle size of the porous media, the type of macrophytes, the clearance kinetics, the transfer of oxygen and the structure and metabolism of the biofilm. The development and application of process-based numerical models made possible simulating a large number of physical, chemical and biological processes that occur in parallel and affect each other. By representing the conditions in terms of flow and transport of pollutants, numerical models allow to simulate the CWs behavior for long-term forecasts and for the time life evaluation. The models could also help to improve the engineering design and the effects of processes as the clogging in porous media. This paper presents the state of the art on the application of numerical model to simulate flow, transport and transformation/degradation of pollutants in subsurface flow constructed wetlands, highlighting, also, the Brazilian's research experience on that.

NUMERICAL SIMULATION IN SUBSURFACE FLOW CONSTRUCTED WETLANDS

The application of numerical models for CWs simulation system allows to describe the processes in progress (such as water flow and oxygen transfer) and to compare the performance between similar systems and their behavior under different conditions (such as the effect of loading quality, different plant species or the seasonality). Also, makes possible to predict the performance of a system for the improvement of the design and to assist in operational control.

The following factors, related to modeling, affect the biochemical transformation and degradation processes in the CWs systems: the microbial community (with the resulting biofilm), the vegetation (influence the water balance, the oxygenation and the nutrient cycling) and the physical properties (porosity, hydraulic conductivity and the particle size of the porous media) (Langergraber, 2001).

Different authors highlight the contribution of each one of the intervening factor. For some authors, biological processes, originated from microbial metabolism, are considered a key to describe the overall operation of the CWs (Samsó & García, 2013; Campà, 2014). On the other hand, some authors highlight the importance of identifying the influence of water distribution mechanisms in order to better understand the systems performance (Brovelli *et al.,* 2007). On that matter, they believe that for a good model calibration the hydraulic properties of the porous media have more influence than the biokinetic parameters, since for reactive transport simulation there is already a good set of experimental biokinetic data to be used as input parameters (Langergraber, 2001).

Models to simulate subsurface flow in SSF-CWs can being classified into the following groups: (a) flow and biokinetic reactions models: for saturated flow (Brovelli *et al.,* 2007; Ojeda *et al.,* 2008) and for variable saturated flow (Langergraber & Šimůnek, 2005; Langergraber *et al.,* 2009; Giraldi *et al.,* 2010); (b) models for a single process or phenomena: to simulate degradation/transfer of a compound or a family compounds (such as organic matter, total nitrogen, oxygen, etc.), and; (c) models to support CWs design: for improving the engineering projects approach. In this study, we present the state of the art on the use of software for flow and biokinetic reaction simulations, in saturated and variable saturated subsurface flow constructed wetlands (**Table 1**).

Among the software selected, FITOVERT is the only one that does not use the biokinetic models Constructed Wetlands 2D (CW2D) or Constructed Wetlands Model 1 (CWM1). This software is based on the mathematical formulation of the IWA Activated Sludge Models (ASM) (Henze *et al.,* 2000), including fractions of organic matter and nitrogen.

The CW2D software is based on the mathematical formulation of the ASM and is specifically designed to simulate the most common processes in VSSF-CWs, including dissolved oxygen (O_2), three fractions of organic matter (readily and slowly biodegradable and inert), four compounds of nitrogen (NH_4, NO_2, NO_3 and N_2N), inorganic phosphorus, heterotrophic microorganisms (considered responsible for hydrolysis, mineralization of organic matter and denitrification) and autotrophic microorganisms (considered responsible for nitrification).

The CWM1 software is based on the mathematical formulation of the ASM and the Anaerobic Digestion Model (ADM) (Batstone *et al.,* 2002) and include fractions of organic matter, O_2, NH_4, NO_2, NO_3, in addition to sulfur fractions (SO_4 and H_2S) and fermentation products. The model can be applied to HSSF-CWs and VSSF-CWs.

FITOVERT

FITOVERT is a 1D model developed in MATLAB (MathWorks Corp®) specifically for descending flow VSSF-CWs simulation, only in one-dimensional flow from the top to the base of the system, neglecting horizontal flows. The software is able to process the flow of water through a variably saturated porous media. Also, considers the effect of evapotranspiration, besides simulating the transport of dissolved and particulate compounds.

The clogging can be simulated as a reduction of porosity on the porous media by modifying the hydraulic conductivity, on the modified Carman- Kozeny equation (Boller & Kavanaugh, 1995). One limitation is that the model does not considers the adsorption of pollutants and the uptake of nutrients and metals by plants (Campà, 2014; Giraldi *et al.,* 2010).

The performance of FITOVERT was evaluated through the verification model. Modeling results were compared with hydrodynamic field tests resulting from a pilot project of VSSF-CW (Giraldi *et al.,* 2010). The VSSF-CW was built with 33 m² of surface area and 68 cm depth, fulfill with six gravel layers and planted with *Cyperus papyrus*, *Canna* sp., *Iris pseudacorus*, *Phragmites australis* and *Juncus ensifolius*. The hydrodynamic tests were performed by using tracers in three different saturation conditions: fully saturated, partially saturated and completely drained. According to the results, the FITOVERT proved to be able to accurately simulate the hydraulic behavior of the studied system in saturated and unsaturated conditions. However, there is still necessary to run additional experiments on the relationship between dispersibility and degree of saturation, to improve the input data for the mathematical models. That can help on the model calibration, based on reliable data of biochemical and transportation processes.

HYDRUS-CW2D

The CW2D (Constructed Wetlands 2D) consists on a biokinetic model of reactive transport simulation with biochemical degradation and transformation processes, developed as an extension of HYDRUS-2D (PC-Progress®). The nitrification is simulated as a two-step process (from ammonia to nitrite and after that, to nitrate), based on ASM (Henze *et al.,* 2000) and other formulations (Nowak, 1996; Brouwer *et al.,* 1998).

As a limitation, HYDRUS-CW2D only considers dissolved compounds, making unsuitable for researching clogging phenomena (García *et al.,* 2010). In addition, takes as a constant the microorganisms concentration in each finite element and do not consider the thickness of the biofilm (Langergraber, 2001).

Table 1. Software for flow and biokinetic reaction simulations in subsurface flow constructed wetlands (SSF-CWs)

Main characteristics		Software FITOVERT	HYDRUS-CW2D	HYDRUS-CWM1	CWM1-RETRASO	PHWAT
Simulation Platform		MATLAB	HYDRUS-2D	HYDRUS-2D	*RetradoCodeBright*	PHWAT
Biokinetc model		Their Own	CW2D	CWM1	CWM1	CW2D
Dimension		1D	2D	2D	2D	1D, 2D and 3D
Availability		No	commercialized	commercialized	Free of charge	Free of charge for noncommercial use
Numerical method		Finite elements	Finite elements	Finite elements	Finite elements	Finite differences
Hydraulic and hydrodynamic	Saturation	Variably saturated	Variably saturated	Variably saturated	Saturated	Saturated
	HSSF-CWs / VSSF-CWs	VSSF-CWs	VSSF-CWs	VSSF-CWs / HSSF-CWs	HSSF-CWs	HSSF-CWs
	Feed	Feeding-emptying cycles	Batch	Continuous	Continuous	-
	Clogging	Yes	No	Yes	Yes	Yes
Biokinetic	Types	C, N and O	C, N, O and P	C, N, O and S	C, N, O and S	C, N, O and P
	Functional bacterial groups	-	3	6	6	3
	Bacterial growth	Yes	Yes	Yes	No	Yes
	Biomass	Attached	Attached	Attached	Suspended	Attached / suspended
	Growth limitations	Substrates	Temperature and substrates	Temperature and substrates	-	Temperature and substrates
Physico-chemical		Atmospheric oxygen transfer, gas transport, transport of particulate components and filtration	Atmospheric oxygen transfer, gas transport and sorption	Atmospheric oxygen transfer, gas transport, transport of particulate components and sorption	Atmospheric oxygen transfer, gas transport, chemical equilibrium and transport of particulate components	Atmospheric oxygen transfer, gas transport, pH, redox, chemical equilibrium, transport of particulate components and attachment/detachment of biomass
Main publications		Giraldi *et al.* 2010	Langergraber & Šimůnek (2005), Morvannou *et al.* (2014)	Langergraber *et al.* (2009), Rizzo *et al.* (2014), Pálfy & Langergraber (2014)	Ojeda *et al.* (2008), Llorens *et al.* (2011*a*), Llorens *et al.* (2011*b*)	Brovelli *et al.* (2007), Brovelli *et al.* (2009)

HYDRUS-CW2D code was verified base on a data set from two VSSF-CWs constructed on a pilot scale (both of them with 1 m² of surface area, filled with 60 cm of sand) (Langergraber & Šimůnek, 2005). The numerical model was calibrated for reactive transport of a single and multiple components. According to the authors, the calibration showed accuracy between the model results and the experimental data.

A research, applied HYDRUS-CW2D to simulate a French type of VSSF-CW, with 28 m² of surface area, filled with gravel and a surface sludge layer of 20 cm and grown with *Phragmites australis* (Morvannou *et al.,* 2014). The system, applied to the treatment of domestic wastewater, was fed with batches for 3.5 days and then rested 7 days. In addition to the hydraulic and biokinetic parameters, the model input included the ammonium adsorption coefficient. The software was applied to simulate the concentration of oxygen, biomass, COD, ammonium and nitrate in the effluent. One of the conclusion of the research was that, during the feeding period, the ammonium was significantly adsorbed in the organic matter being oxidized to nitrate during the rest of the period.

Numerical models have being applied successfully to simulate subsurface flow and biokinetic reactions in constructed wetlands. To select the software to simulate SSF-CWs systems is needed take into account the degree of saturation and the flow direction (the hydraulic and hydrodynamic of the porous media). The CWM1-RETRASO and PHWAT codes are suitable only for saturated conditions, while FITOVERT, HYDRUS-CW2D and HYDRUS-CWM1 run simulations for variably saturated conditions.

The HYDRUS-CWM1 is the only one that has been calibrated for both systems, HSSFS-CWs and VSSF-CWs, showing good simulations results. Among the software, the HYDRUS-CW2D simulates only dissolved components, being the only one unable to reproduce the effects of clogging.

To the simulation of VSSF-CWs system, the FITOVERT code shows being a simplistic model, providing friendly use with fewer input data requirement. However, FITOVERT is restricted to 1D simulations and limited to the modeling of organic matter, nitrogen and oxygen, without including the transformation of S or P. A complete 2D simulation of VSSF-CWs can be made through HYDRUS-CW2D model, in the case of available data, since the software input includes more species and additional processes such as adsorption of ammonia.

In the case of HSSF-CWs systems, both HYDRUS-CWM1 and CWM1-RETRASO run 2D simulations, taking into account the same species (C, N, O and S) and a similar number of reactions (17 and 19, respectively). An important difference between them is that CWM1-RETRASO is unable to simulate the effects of transpiration and ignores the limitations of bacterial growth, while the HYDRUS-CWM1 is able to simulate the effects of transpiration and the limitations of growth caused by the temperature and the substrate. To simulate P in HSSF-CWs, the only applicable software is the PHWAT, but it is difficult to calibrate.

About the biokinetic processes, stand out the HYDRUS-CWM1 model, because can simulate the attached biomass, and the PHWAT model because can simulate attached and suspended biomass. Besides the transport of dissolved and suspended species, PHWAT is able to account for growth-limiting expression, caused by factors related to temperature and the substrate. About the physical and chemical processes, the PHWAT is the most complete software, the only one that includes the production of gases generated on the treatment process.

All the software were calibrated with data from a CW's experimental system or a real scale CW's project (ranging from 28 m² for VSSF-CW simulated with HYDRUS-CW2D, to 55 m² for HSSF-CW simulated with CWM1-RETRASO). Most of the projects have used gravel as porous media and were vegetated with *Phragmites australis*.

In Brazil, very few studies address the subject of CWs simulation. This highlights the need to study CWs performance under Brazilian environments to take into account local factors as wastewater quality, climate, microorganism, plants and local alternatives for porous media.

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