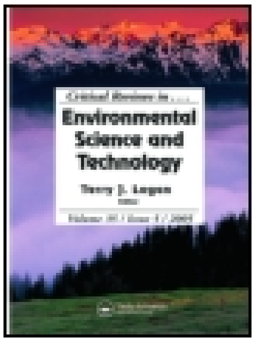

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Modelling approaches for simulating wetland pollutant dynamics

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ABSTRACT
A number of black box and process-based modelling approaches, their strengths/limitations, and future applications for simulating contaminant dynamics in constructed wetlands (CWs) have been reviewed. Scanning of literature reveals that most of the CW modelling approaches are limited to the simulation of only nutrient and organic pollutant load dynamics. Performance analysis of the various process/black box-based models for simulating pollutant dynamics in vertical subsurface flow, horizontal subsurface flow, and hybrid CW systems further reveals that most of the existing modelling approaches have not not so far been able to account for the changing climatic conditions and the heavy metal dynamics. The paper thus highlights the gaps in the knowledge in the current state of the art for simulating wetland pollutant dynamics and suggests mechanisms for increasing the scope of such modelling approaches in the proper design and operation of the CW systems.

KEYWORDS
Constructed wetlands; modelling; pollutants dynamics

1. Introduction

In recent years, water availability has become an issue of global concern. Ever increasing population coupled with industrial and agricultural activities has resulted in the rising demand for good quality water coupled with increased wastewater generation. A number of global water availability assessments have been carried out and many projections and scenarios for future water supply and demand have been formulated. In the last four decades, the number of countries experiencing water scarcity has increased (Kivaisi, 2001). Apart from the global natural freshwater scarcity, the quality of the available freshwater resources is also on a decline due to increased pollution, further intensifying the water shortage problem (Saxena et al., 2016).

Wastewater reuse in agriculture is an important strategy for conserving water resources, particularly in areas suffering from water shortage (Kivaisi, 2001;

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Mthembuet al., 2013). Recycling of treated wastewaters also contributes to environmental protection and reduction in the spread of waterborne diseases (Lan et al., 2010; Akpor and Muchie, 2011; Kumar et al., 2014). Thus, reuse of treated effluents in agriculture for supplemental irrigation is fast becoming popular worldwide for minimizing water scarcity impacts.

Conventional sewage treatment is costly, generates sludge, and requires regular maintenance. Hence, it may not be a suitable strategy for small towns/villages and developing countries. CWs – the engineered wastewater treatment systems, that are based on the optimized treatment processes found in the natural environment (Kadlec and Knight, 1996; Langergraber, 2011), represent sustainable alternatives as they are low cost, easy to use, and eco-friendly (Garcia et al., 2010). Wetlands, comprising of essential structural components such as the planted vegetation (Mitch, 2002; Mairi et al., 2012); microorganisms (Kuiper et al., 2004; Kumar et al., 2011; Mairi et al., 2012); and the substrate viz., sand, soil, and/or gravel (Kuiper et al., 2004; Fonkou et al., 2011), have a natural capacity to remove several types of pollutants e.g., nutrients (N, P), total suspended solids, organic compounds, pathogens, and heavy metals (Vymazal et al., 1998; Kadlec et al., 2000; Vymazal, 2005; Garcia et al., 2010). The pollutant removal in CWs is facilitated through a combination of physical, chemical, and biological processes including sedimentation, precipitation, adsorption, and assimilation through the combined action of the substrate, plant tissues, and microbial transformations (Garcia et al., 2010; Marchand et al., 2010, Langergraber 2011, Meyer et al., 2015).

The increased use of CWs for wastewater treatment in different countries, coupled with increasingly strict water quality standards, has been a motivation for the development of better modelling approaches as design tools (Rousseau et al., 2004). Available CW models can primarily be grouped into two types viz., black box (i.e., empirical/statistical) and process based. Contrary to the process-based models, that take into account various physical, chemical, and biological processes, the black box models do not describe a process. Thus, black box modelling approaches fail to account for the inherent complexity of the processes operative in the CWs. In recent years, both these modelling approaches have been investigated and reviewed extensively by a number of researchers (Langergraber, 2008; Garcia et al., 2010; Kumar and Zhao, 2011; Samso and Garcia, 2013a, b; Samso, 2014; Meyer et al., 2015). However, scanning of literature reveals the need for a consolidated review on the range of the contaminant removal processes accounted for by the existing models, their assets/limitations, and future considerations for improving their application potential in different types of CW systems. Hence the present study aims to investigate and present these aspects in the following sections.

2. Black box models

In CWs a large number of physical, chemical, and biological processes are operative in parallel, which mutually influence each other. Therefore for a long time, CWs have been considered as 'black boxes' based on a number of simple and advanced regression modelling methods. In fact a number of regression equations have been modelled so far to predict outflow concentrations of the CWs as a function of their inflow concentrations and hydraulic loading rates. These equations, as proposed by different authors, have been extensively reviewed by Rousseau et al. (2004) for the horizontal subsurface flow (HSSF) treatment wetlands. Table 1 illustrates a variety of such regression models developed for estimating the removal of different pollutants through CWs (Tang et al., 2009; Son et al., 2010). Investigations reveal that though these models can predict output data as a function of the input data, with a high (70%) coefficient of variation they are incapable of explaining any internal pollutant removal processes. The following sections illustrate some key attributes of each of these black box modelling approaches.

2.1. First-order models

A number of non-linear deterministic models for predicting pollutant outlet concentrations of CWs, based on their inlet concentrations, have been proposed (Kadlec and Knight, 1996; Kadlec, 2000; Stone et al., 2004; Stein et al., 2007; Sun et al., 2008; Kadlec and Wallace, 2009). Kumar and Zhao (2011) illustrated that many wetland processes viz., mass transport, volatilization, sedimentation, and sorption are basically first-order and hence can be best expressed through the

Table 1. Regression equations for constructed treatment wetlands according to different authors.

Country	Type of CW	Regressors	Predictor parameter	equations	R^2	References
US	SSF	Lin (BOD)	BOD (Lremoved)	Lremoved = 0.653 ∗ Lin + 2.92	0.97	Reed and Brown (1995)
Szech Republic	SSF	Lin (BOD)	BOD (Lout)	Lout = 0.145 ∗ Lin − 0.06	0.85	Vymazal (1998)
Szech Republic	SSF	Lin (COD)	COD (Lout)	Lout = 0.17 ∗ Lin + 5.78	0.73	Vymazal (1998)
China	IVSF	T, pH	NO3-N	2.942T − 22.530pH + 169.05	0.706	Chang et al (2013)
Greece	VF	COD, NH3-N	TKN	$C_{TKNout} = 0.042 * C_{CODin} + 0.823 * C_{NH3\text{-}Nin} + 8.878$	/	Gikas et al. (2011)
Greece	VF	TSS, DO, EC, COD	TSS	$C_{TSSout} = 0.245 * C_{CODin}\text{-}0.043 * C_{ECin}\text{-}8.097 * C_{DOin} + 93.540$	/	Gikass et al. (2011)
United Kingdom	SSVF	EC, pH, EC, redox, T and DO	Benzene	Benzene = 1413.57 + 16.33DO + 0.04EC + 0.28redox − 204.36pH − 2.69T	0.748	Tang et al. (2009)
		BOD influent, q	BOD effluent	$C_{out} = 0.6249 C_{in}^{1.1012} q^{0.0562}$	0.53	Son et al.(2010)
		TP influent, q	TP effluent	$C_{out} = 0.3857 C_{in}^{0.9621} q^{0.0.2175}$	/	Son et al. (2010)

The nomenclature used in the Table 1 is as follow: SSF = Subsurface Flow; HSF = Horizontal Surface Flow; SSVF = Subsurface Vertical Flow; IVF = Integrated Vertical Flow; Lin/out/removed = input/output/removed BOD normality loads; DO = Dissolved Oxygen (mg/l); COD = Chemical Oxygen Demand (mg/l); C_{DOin} and C_{ECin} = input concentrations of DO and EC respectively; C_{CODin} = COD input concentration; BOD = Biochemical Oxygen Demand (mg/l); TSS = Total Suspended Solids (mg/l); $C_{TSSout/in}$ = Output/input Total Suspended Solids concentration (mg/l); EC = Electrical Conductivity (μS/cm); T = Temperature (°C); TP = Total Phosphate (mg/l); TKN = Total Kjeldhal Nitrogen (mg/l); $C_{TKNout/in}$ = Output/input Total Kjeldhal Nitrogen concentration (mg/l).

following first-order equations:

$$\frac{Cout}{Cin} = e^{-kA/q} \tag{1}$$

or

$$\frac{Cout}{Cin} = e^{-kvT} \tag{2}$$

Where, C_{in} (mg/m^3) is the inlet concentration, C_{out} (mg/m^3) is the outlet concentration, kA is a real decomposition constant (d^{-1}), q isthe hydraulic loading rate (HLR in md^{-1}) while kv is the volumetric decomposition constant (d^{-1}) and T is the hydraulic retention time (HRT) in days. Another modified first-order kinetic model, often called the $k - C^*$ model, introduced by Kadlec and Knight (1996) has also been widely applied in the CW designing, wherein the non-dispersive flow conditions (i.e., plug flow reactor conditions), are expressed as:

$$\frac{C - C^*}{Ci - C^*} = e^{-ky/q} \tag{3}$$

or

$$\frac{C - C^*}{Ci - C^*} = e^{[-Kv\tau y]} \tag{4}$$

Where, C_i is the inlet concentration (mg/m^3), q the HLR (in md^{-1}), C^* is the background concentration (mg/m^3), y *is* the fractional distance through the wetland (x/L), L is the wetland length (m), and τ is the nominal detention time in days (d).

Analysis of the above-mentioned first-order rate constants (k) worked out by Rousseau et al. (2004) and Garcia et al. (2010) for the various HSSF CWs has shown that these rate constants are in reality not constant but vary with varying effluent concentrations, HLRs, and water depths (Kadlec, 2000). These were also found to be a function of the void fractions, wetland age, background pollutant concentrations (C*), plant species, and temperature (Rousseau et al., 2004; Stein et al., 2007). Goulet et al. (2001) tested the suitability of the first-order models for predicting metal retention in a young CW receiving agricultural and urban runoff. Investigations revealed that these models could give realistic estimates of iron (Fe) and manganese (Mn) retention, during spring, and of zinc (Zn) retention from spring to fall but failed to fit summer, fall, and winter data for almost every metal under investigation (e.g., Fe, Mn, copper, and arsenic), thereby suggesting that HRTs (from 1 to 25 days) did not affect metal retention during these seasons.

2.2. Monod models

In biological systems, the degradation rates are in general limited by the availability of pollutants at lower concentrations and are saturated at relatively higher pollutant concentrations (Mitchell and McNevin, 2001). Hence, as evident from the following equation:

$$r = ko, v * V \frac{C}{K_{HSC} + C} \tag{5}$$

Where, r (mg/d) is the rate of biological degradation, K_{HSC} (mg/m^3) is the half-saturation constant, C is the contaminant concentration (mg/m^3), ko,v is the zero-order volumetric rate constant (mg/m^3/d), and V is the pore volume (m^3); when C is far less than K_{HSC}, first-order kinetics prevails while as C increases, the kinetics becomes zero-order kinetics (Langergraber and Simunek, 2005). As a result, due to low reaction rates at lower concentrations, such modelling approaches prevent total decomposition of pollutants and are thus often associated with a residual outlet concentration C^* (mg/m^3). Hence Monod equations have been observed to be very useful for representing transition of any first-order process to the zero-order biological degradation kinetics (Kumar and Zhao, 2011) and therefore have often been observed to describe well the observed wetland performance, particularly in terms of their biochemical oxygen demand (Mitchell and McNevin, 2001; Sun et al., 2008).

2.3. Time-dependent retardation model

As easily biodegradable substances are removed first and faster, and thereby leave a solution with less biodegradable constituents and slower removal kinetics, in CWs the pollutant removal rates in general decrease as a function of time (Shepherd et al., 2001). Kumar and Zhao (2011) also illustrated that a continuous change in wetland solution concentration can be best represented through the following time-dependent volumetric first-order rate constant, k_v:

$$k_v = \frac{k_0}{(b\tau + 1)} \tag{6}$$

Where, k_0 is the initial first-order rate constant (d^{-1}), b is the time-based retardation coefficient (d^{-1}), and τ is the retention time (d). It has been observed that this approach is the most appropriate for the CW designing as it allows a steady decrease in the pollutant concentration with increased treatment time, rather than leading to a constant residual concentration.

Shepherd et al. (2001) introduced the aforementioned modelling approach for simulating chemical oxygen demand (COD), removal across different depths and at different loading rates in a pilot-scale CW designed for treating high-strength winery wastewater, and compared its efficiency against the earlier modelling approaches to show that the two-parameter residual ($K - C^*$) and retardation ($K - b$) models could fit the measured pollutant removal concentrations better than the single-parameter first-order decay model. However, such modelling approaches require tracer studies for computing the aforementioned pollutant removal rate constants.

2.4. Tanks-in-series model

The Tanks-In-Series (TIS) model, developed by Kadlec (2003), basically characterizes the discharge of the pollutant at the outlet as it traverses through the wetland as a function of the detention time distribution (DTD). Kadlec and Knight (1996) observed that the detention time is in general variable along the wetland and is a function of the vegetation density, topography, and other environmental factors. In the TIS modelling approach, a wetland is normally divided into '*N*' number of same-sized compartments, where the concentration of a pollutant leaving each tank is considered to be equal to the uniform internal concentration in that tank (Kadlec and Knight, 1996; Mietto, 2009). A number of mechanistic models, such as TIS and plug flow (PF) with dispersion, have been utilized to describe wetland DTD (Kumar and Zhao, 2011). However, the most common of these is the TIS model expressed as the following gamma distribution function:

$$g(t) = \frac{1}{(N-1)!\mathrm{t_i}}\left(\frac{t}{t_i}\right)^{N-1}\left(\exp^{\frac{\mathrm{t}}{\mathrm{t_i}}}\right) \tag{7}$$

Where, t is the detention time in days (d), t_i is the mean detention time in one tank (d), and N is the number of tanks. Although the TIS mixing can be described through the gamma distribution it cannot address turbulent mixing, if any, within the wetlands (Khan, 2011). Further, the TIS models are focussed only on the input/output data rather than the internal process data.

Udameri (2009) and Khan (2011) used the TIS model to characterize the movement and discharge of the pollutants at the outlet of a wetland. Krone–Davis et al. (2013) also applied the TIS modelling approach to simulate the degradation of three highly water-soluble pesticides (e.g., diazinon, methomyl, and acephate) by a full-scale constructed treatment wetland located at the base of the Salinas Valley. The investigations revealed that the confidence intervals for the first-order decay rates (ranging between 0.097 and 0.289 day^{-1} for diazinon, 0.068 and 0.232 day^{-1} for methomyl, and 0.068 and 0.246 day^{-1} for acephate) computed by the TIS approach can be successfully used, in conjunction with the simple decay models, to optimize the design of wetlands and to estimate their size requirements.

2.5. Artificial Neural Networks (ANN)

An ANN, also called Neural Network (NN), is a computational method that simulates the structure and/or functional aspects of the biological neural networks or recognizes and simulates the pattern and process in many areas of science and technology (Nayack et al., 2006; Nayak et al., 2006; Naz et al., 2009). Akatros et al.

(2009a, b) derived the following design equation, through the ANN approach, for the removal of total nitrogen (TN) from CWs:

$$R_{TN} = \frac{HRT}{K_{TRSP} + HRT} \tag{8}$$

Where,R_{TN} is the TN removal, HRT is the hydraulic retention time in days (d), and is the time scale of the removal process in days (d) as expressed through the following equation:

$$K_{TRSP} = \left(\frac{22.8}{T}\right) 45.5 \left(\frac{n}{n-1}\right)^3 \tag{9}$$

Where, n is the porosity of the media and T is the wastewater temperature (in °C).

As an alternative to the first-order model, the aforementioned design equation for TN removal has been applied to even model phosphorus removal, predict hydraulic conductivity (Kumar and Zhao, 2011), and assess NH_3 removal from the HSSF and the Free Surface Water CWs (Naz et al., 2009). Yakul (2013) successfully applied an ANN model to even estimate phenol removal from the pilot-scale vertical and horizontal CWs.

Comparative performance analysis of the multiple regression analysis and the two ANNs – Multilayer Perceptron and Radial Basis Function network models, for predicting biochemical oxygen demand (BOD) (Tomenko et al., 2007) illustrated the superior performance of the ANN models. Zare (2014) also compared the predictive efficiency of the multivariate linear regression (MLR) and the ANN models for the COD and BOD removal from the constructed treatment wetlands to reveal that ANN models have an edge over the MLR approaches. Lee et al. (2011) suggested a sequential modelling approach, using ANNs, to develop four independent multivariate models that could realistically predict the COD, BOD, suspended solids (SS), and TN removal from the CWs. Self-Organizing Map, a type of ANN model, has also been developed and successfully validated for predicting BOD, NH_3-N, P, and heavy metal removal from the CWs.

3. Process-based models

As process-based models (Table 2) are based on an increased understanding of the processes involved in pollutant transfer within CWs (Langergraber, 2007; Garcia et al., 2010; Meyer et al., 2015), such approaches can lead to effective wetland designing. The process-based models normally use Richards equation or other simplified approaches to describe various wetland processes, such as variably saturated water flow, convective–dispersive transport in liquid phase, diffusion in gaseous phase, adsorption–desorption processes in solid/liquid phases, biokinetics of

Table 2. Types of softwares and models related to different processes simulated in constructed wetlands.

		Types of sub-models related to processes			
N0	Designation (software/model)	Hydraulic and hydrodynamic processes	Biokinetic processes	Physico-chemical processes	Main references
1	FITOVERT (Software)	- Richards/Transport equations - Evapotranspiration - Clogging process - Surface flow	- C, N, O - Bacterial growth, - Biomass description - Monod type	- Atmospheric oxygen transfer - Gas, particles and particulates transport - Filtration	Brovelli et al. (2007), Giraldi et al. (2010)
2	Activated Sludge Model (ASM)	No	Yes, biokinetic model	No	Henze et al. (2000)
3	Constructed wetland Two-Dimensional (CW2D) model	No	Yes, biokinetic model, based on a mathematical formulation of the ASM models	No	Langergraber (2001), Langergraber and Šimunek (2005)
4	PHREEQC (Software)	—	- Aerobic processes based on CW2D, - C, N, P - Monod-type	- Mineral and gas mole transfer, sediment–water interactions	Claveau-Mallet et al. 2012, 2014
5	PHWAT (Software)	- Darcy/Transport equations - Clogging process	- C, N, P, O - Monod type (CW2D) - 3 functional bacterial groups - Bacterial growth, biomass description	Atmospheric oxygen transfer - Gas, particle and particulates transport - pH, redox, chemical equilibrium, - Filtration/sedimentation: Attachment or detachment to biomass	Brovelli et al. (2007, 2009a, b, c), Mao et al.(2006), Samo et al. (2014b)
6	CWM1(Constructed Wetland Model No.1)	No	Biokinetic model Constructed Wetland Model Number 1 (CWM1) to describe biochemical transformation and degradation processes for organic matter, nitrogen and sulphur in subsurface flow constructed wetlands	No	Langergraber et al. (2009a)
7	2 D HYDRUS/CWM1 (HYDRUS Wetland Module)	- Richards/Transport equations - Transpiration - Surface flow	- C, N, P, O - Monod type (CWM1) - 3 functional bacterial groups - Bacterial growth, biomass description	- Atmospheric oxygen transfer - gas transport - Sorption processes	Palfy and Langergraber, 2014 Rizzo et al. 2014

8	HYDRUS/CW2D (HYDRUS Wetland Module)	- Richards/Transport equations - Evapotranspiration - Surface flow	- C, N, P, O - Monod type (CW2D) - 3 functional bacterial groups - Bacterial growth, biomass description	- Atmospheric oxygen transfer - gas transport - Sorption processes	Langergraber and Simunek (2005, 2013), Langergraber (2013), Morvannou et al. (2013), Garcia et al. (2010)
9	BIO_PORE (Software)	-Darcy/Transport equations	- C, N, O, S - Monod type (CWM1) - 6 functional bacterial groups - Bacterial growth, biomass description (attached)	- Atmospheric oxygen transfer - Filtration - Transport of particulates components	Samso and García, (2013a,b)
10	Retraso Code Bright (RCB) flow model	-Darcy's and Fick's laws	- Organic matter, nitrogen and sulphur transformation processes	- Advection, dispersion and diffusion - Reactive transport of inorganic dissolved and gaseous species	Ojeda et al. (2009)
11	STELLA(Structural Thinking Experimental Learning Laboratory with Animation) (Software)	Variably saturated conditions	- Nutrient and organics removal, microbial degradation (dynamic), plant uptake (dynamic)	Adsorption, desorption	Wang and Mitsch (2000); Ahn and Mitsch (2002a); Ouyang et al. (2010)
12	Wang-Scholz-Model(COMSOL)	Darcy's law Clogging processes	/	- Liquid-solid mixture, diffusion process, sedimentation and adsorption	Sani et al. (2013)
13	1 D-Diph_M (MATLAB)	Unsaturated (two-phase flow)	Forms of COD, NH_4-N, oxygen	No	Petitjean et al. (2012) Forquet et al. (2009a, b); Mayer et al. (2015)
14	AQUASIM-CWM1 (AQUASIM Software)	Tanks in series with saturated water content	- C, N, P, O, S - Monod type (CWM1) - 6 functional bacterial groups - Bacterial growth, biomass description (suspended)	- Atmospheric oxygen transfer - gas transport - Adsorption/desorption	Llorens et al. (2011a, b)
15	Dual-porosity model (DPM) in HYDRUS-1D (Software)	Saturated, unsaturated and preferential (Richards eq. + dual porosity)	No	- Atmospheric oxygen transfer - gas transport - Sorption processes	Morvannou et al. (2013)
16	CMW1-RETRASO model.	- Darcy/Transport equations	- C, N, O, P - Monod type (CWM1) - 6 functional bacterial groups - Biomass description (suspended)	- Atmospheric oxygen transfer - gas, particles and particulates transport - chemical equilibrium,	Langergraber et al. (2009a)

(*Continued on next page*)

Table 2. (Continued)

		Types of sub-models related to processes			
N0	Designation (software/model)	Hydraulic and hydrodynamic processes	Biokinetic processes	Physico-chemical processes	Main references
17	RTD/GPS-X model	Tanks in series with recycle and dead volumes under variable water content	12 species considered, including forms of COD, N (only soluble), Interaction with biofilm growth	No	Zeng et al. (2013a)
18	RSF_Sim	Tanks in series with variable water content	- C, N, P (In progress) - Sediment accumulation description	- Particles and particulates transport - Filtration/Sedimentation - Sorption processes	Dittmer et al. (2005), Henrichs et al. (2007, 2009), Meyer et al. (2006), Pálfy and Langergraber (2014), Meyer et al. (2013).

pollutant transformation and degradation, root growth/decay, plant uptake, release of specific organic substances and oxygen, and transport/deposition of suspended particulate matter (Langergraber, 2017). Some of the most commonly used models, based on the aforementioned processes, are illustrated in the following sections:

3.1. Activated sludge model (ASM)

In CWs, the decomposition of biodegradable organic compounds is based essentially on the aerobic or anaerobic microbial activities (Henze et al., 2000). As these microbial activities on organic compounds are well captured in the functional system of the ASM, the ASM1 (Henze et al., 1987) and the ASM2 (Henze et al., 1995) are still considered to be state-of-the-art models for the dynamic simulation of not only biological COD but also biologic N and P removal from the activated sludge systems. The ASM primarily comprises of 3 components viz., the biomass, substrate, and the dissolved oxygen (DO). Besides, it takes into consideration two processes viz., the aerobic and the anoxic, leading to the growth and decay of the biomass. The kinetics or the rate equations explaining biomass growth are based on the Monod equations whereby the biomass growth is considered to be proportional to the biomass concentration, in a first-order manner and to the substrate concentration, in a mixed-order manner. In contrast, the biomass decay is explained by the Monod–Herber equation (Giraldi et al., 2010) whereby the biomass decay is considered to be a first-order process with respect to the biomass concentration.

3.2. FITOVERT model

The FITOVERT model which is also the FITOVERT Wetland module developed on FITOVERT software is a numerical multicomponent reactive transport model (Giraldi et al., 2010) specifically developed to simulate and forecast the behaviour and treatment properties of vertical subsurface flow (VSSF)-CWs under variably saturated conditions. In fact the FITOVERT model has been primarily developed to overcome the deficiencies associated with the so far developed wetland models (Kumar and Zhao, 2011) that can primarily simulate horizontal subsurface flow constructed wetlands (HSSF-CWs). The FITOVERT model basically comprises of the hydraulic and the biochemical modules along with the processes governing dissolved/particulate matter transport, clogging of the wetland system, evapo-transpiration, and oxygen transfer:

In the hydraulic module of the FITOVERT model, the vertical flow of water through the porous media, under unsaturated conditions, is described through the following Richards equation:

$$\frac{\partial \theta}{\partial t} = + \frac{\partial}{\partial z}\left[K\left(\frac{\partial h}{\partial z} - 1\right)\right] \tag{10}$$

Where, θ is the volumetric water content, t is the time (in in seconds), z is the spatial coordinate (in metres; positive downwards), K is the unsaturated hydraulic conductivity (in ms^{-1}), and h is the matrix potential (in m). The volumetric water content (θ) and the unsaturated hydraulic conductivity (K) are in turn expressed through the following van Genuchten–Mualem functions (Van Genuchten, 1980) and the related empirical parameters viz., α (m^{-1}) and m (unitless):

$$\theta = \theta r + \frac{\theta s - \theta r}{\left(1 + |\propto h|^{\frac{1}{1-m}}\right)^{m}}, \tag{11}$$

and

$$K = Ks\left(\frac{\theta - \theta r}{\theta s - \theta r}\right)^{0.5}\left[1 - \left(1 - \left(\frac{\theta - \theta r}{\theta s - \theta r}\right)^{\frac{1}{m}}\right)^{m}\right]^{2} \tag{12}$$

Where, θr and θs are the residual and saturated volumetric water contents, respectively, and Ks (in ms^{-1}) is the saturated hydraulic conductivity.

The processes responsible for the removal of the biodegradable organic matter and the nitrogenous compounds in the FITOVERT model are explained through the ASM1 (Henze et al., 2000), wherein the biodegradation kinetics of the wetland system is expressed through a set of eight Monod-type equations. While the transport of the dissolved components, through advection–dispersion in liquid phase, is expressed through the following Bresler's equation (Bresler, 1973):

$$\theta.\frac{\partial c}{\partial t} = \frac{\partial}{\partial z}\left(d.\frac{\partial c}{\partial z}\right) - q.\frac{\partial c}{\partial z} + R.\theta \tag{13}$$

Where, c is the concentration of the single soluble component in water (in gm^{-3}), d $= \lambda \frac{q}{\theta}$ (15) is the dispersion coefficient (in $m^2\ s^{-1}$; Ogata, 1970), λ is the dispersivity (in m), q is the specific flow rate (in $m^3\ m^{-2}\ s^{-1}$), and R is the reaction term (in $gm^{-3}\ s^{-1}$) as obtained from the biochemical module and the diffusive exchange of the DO (Giraldi et al., 2010).

The transport and filtration of particulate components are described with an original scheme based on the work of Iwasaki (1937), later developed by Ives (1969) for the numerical analysis of the sand filtration process in saturated condition:

$$-q.\frac{\partial Tm}{\partial z} = \theta\frac{\partial Tm}{\partial t} + q.f.Tm \tag{14}$$

Where Tm(gm^{-3}) is the concentration of each single particulate component in water, and f(m^{-1}) is the filter coefficient. FITOVERT handles the porosity reduction due to bacterial growth and filtration of particulate components, by means of a continuous update of the total volumetric specific deposit D_{vtot} ($m^3\ m^{-3}$).

The effect of pore size reduction on the hydraulic conductivity is also considered by the Carman–Kozeny equation (Boller and Kavanaugh, 1995), modified according to O'Melia and Ali (1978). The final formulation leads to a correction term for the hydraulic conductivity:

$$K = \frac{Ko}{\left[\left(1 + p\frac{Dvtot}{\varepsilon o}\right)^{X}\left(1 - p\frac{Dvtot}{\varepsilon o}\right)^{Y}\right]} \tag{15}$$

Where Ko (ms^{-1}) is the hydraulic conductivity for the clean filter; εo (m^3m^{-3}) is the porosity of the clean filter; and p (unitless), × (unitless), and y (unitless) are empirical parameters.

The oxygen transport in liquid phase and other dissolved components are described by means of the same transport equation. Therefore, the reaction term accounts for both the biochemical reactions and the diffusive exchanges with the gaseous phase. The exchanges of oxygen between the liquid and the gaseous phases are modelled according to Fick's law. FITOVERT adopts a global coefficient of oxygen transport K_{la} (s^{-1}), which can vary to account for the reduction of interchange surface due to the increase of water content:

$$K_{la} = \left(1 - \frac{\theta}{\theta r}\right)K_{lao} \tag{16}$$

Where, K_{lao} (s^{-1}) refers to the drained conditions. The oxygen transport in gaseous phase is described by means of a mass balance equation assuming that the diffusion coefficient for oxygen in free air Da (m^2 s^{-1}) is corrected by means of a tortuosity factor (Patwardhan et al., 1988), according to the formulation of Marshall (1959):

$$D = (\mathscr{E} - \theta)^{3/2}D_a \tag{17}$$

Where D_a (m^2 s^{-1}) is the diffusion coefficient for oxygen in the bed and ε (m^3 m^{-3}) is the current porosity.

The evapo-transpiration component in the FITOVERT model is the sum of evaporation from the free surface and transpiration from plants in VSSF-CWs. The two terms are identified according to the leaf area index (Liu et al., 2005; Varado et al., 2006) while the actual evaporation rate is defined according to Lappala et al. (1987):

$$Ea(t) = \begin{cases} KsKr(h)SRES\left(h_{top} - \psi\right) & Ea(t) < Ep(t) \\ Ep(t) & Ea(t) \geq Ep(t) \end{cases} \tag{18}$$

Where, $Ea(t)$ is the actual soil evaporation (m s^{-1}); $Ep(t)$ is the potential soil evaporation (m s^{-1}); Ks is the saturated hydraulic conductivity (m s^{-1}); Kr is the relative hydraulic conductivity (unitless); SRES is the surface resistance (m^{-1}), which is the reciprocal of the distance from the node to land surface; ψ is the pressure potential at soil–atmosphere interface (m); and h_{top} is the pressure potential at the first node on the land surface (m).

FITOVERT model has been demonstrated to accurately simulate the hydraulic behaviour of VSSF-CWs under both saturated and unsaturated conditions and the effects of different macrophytes on the nitrogen removal efficiency (Iannelli et al., 2009). Investigations have revealed further model improvements particularly with respect to better mathematical description of the relationship between dispersivity and saturation degree (Giraldi et al., 2010);). Additionnally, accurate simulation of biological changes within the system and uptake as well as adsorption of the nutrients, metals and persistent pollutants by the plants and planting media are totally neglected in the current version of the FITOVERT model.

3.3. CW2D model

The Constructed Wetland 2-Dimensional (CW2D) model was introduced by Langergraber and Simunek (2005, 2006) for simulating the processes controlling the degradation and transformation of dissolved carbon (organics), nitrogen, and phosphorous (Samo, 2014), under saturated/unsaturated conditions in VSSF-CWs, based on the ASM and Richard equation. The above approach basically requires the definition of the following parameters viz., DO; soluble, recalcitrant, and inert carbon fractions; NH_4, NO_2, $NO_{3,}$ N_2N nitrogen concentrations; and inorganic phosphorus concentration. The organic nitrogen and phosphorous are modelled as a part of the COD, and the temperature dependence of all rate and diffusion coefficients is described using the Arrhenius equation.

Toscano et al. (2009) applied the HYDRUS-2D and CW2D models to simulate the hydraulic behaviour and effluent pollutant concentrations in a pilot-scale two-stage subsurface flow CW for the treatment of municipal wastewaters in Italy. Similarly, in Germany, retention soil filters (RSFs) were developed for assessing and monitoring the performance of CWs for combined sewer overflow treatment (Meyer and Dittmer, 2014) through the combined application of the HYDRUS-2D and CW2D models as RSF_SIM model (Dittmer et al., 2005; Palfy and Langergraber, 2014). In all these approaches, the HYDRUS-2D software was used for describing the flow and (single) solute transport, while the multicomponent CW2D model was used for simulating the degradation and transformation of organic matter, nitrogen, and phosphorus. Recently, to facilitate an integrative use of HYDRUS-2D and CW2D models, a yet another multicomponent reactive transport model named HYDRUS-2D-CW2D has been developed (Langergraber and Simunek, 2005, 2012) for simulating the removal of organics and nutrients from CWs under saturated and unsaturated conditions. Though the validation of the aforementioned models, through tracer experiments, has revealed a realistic simulation of water flow and pollutant removal processes it has been observed that this modelling approach is limited to the degradation and transformation of only dissolved pollutants under aerobic/anoxic conditions and hence is not applicable to the CWs in which anaerobic processes play a significant role (Langergraber and Simunek, 2012).

3.4. PHREEQC model

The PHREEQC model is a biokinetic module developed on the PHREEQC software. In this model (Parkhurst and Appelo, 1999), the biochemical reactions controlling various aerobic processes are based on the CW2D model while those controlling anaerobic processes are based on the Maurer and Rittmann (2004) formulations. As the PHREEQC model and its other versions are based on an ion-association aqueous model and has capabilities for speciation and saturation-index calculations, batch-reaction and one-dimensional (1D) transport calculations involving reversible reactions (which include aqueous, mineral, gas, solid-solution, surface-complexation, and ion-exchange equilibrium), and irreversible reactions (which include specified mole transfers of reactants, kinetically controlled reactions, mixing of solutions, and temperature changes), and inverse modelling (which finds sets of mineral and gas mole transfers that account for differences in composition between waters, within specified compositional uncertainty limits) the PHREEQC model and its versions can be used for simulating a variety of reactions and processes in natural waters or laboratory experiments.

3.5. PHWAT model

The PHWAT model is a wetland module developed using the PHWAT Software. According to Brovelli et al. (2009a), the PHWAT model is a numerical model that can be used for simulating pH variations, and the redox and surface-complexation reactions associated with the nutrients and organic pollutants through the integrated use of the latest version of the PHREEQC-2 and the Groundwater Flow model named MODFLOW. The MT3DMS component – a mass transport module (Zheng and Wang, 1999) of the PHWAT model (where MT3D stands for the Modular 3-Dimensional Transport model and MS denotes the Multi-Species structure) is capable of simulating advection, dispersion/diffusion, and chemical reactions of contaminants in groundwater flow systems under varied hydro-geologic conditions based on the standard finite-difference method, particle-tracking based on Eulerian–Lagrangian methods, and the higher order finite-volume transport solution techniques. Though, the PHWAT model is also capable of simulating bio-clogging, bacteria attachment, and flow-induced biofilm detachment (Samso et al., 2014) and has shown reasonably good agreement with the experimental data it has been reported to have limited capability to simulate reduction in porosity due to bacterial growth (Brovelli et al., 2009a). Further its calibration has been found to be extremely difficult, due to the strong non-linearity of the mathematical model.

3.6. BIO-PORE model

Samso and Garcia (2013a) indicated that the name BIO-PORE Model (BIO_PORE wetland module developed in BIO_PORE software) was inspired by the biofilm sub-model. In fact, the Constructed Wetland Model No.1 (CWM1) biokinetic model is implemented to describe the transformation and degradation processes of organic matter, nitrogen, and sulphur. According to the same authors, small changes of CWM1 equations were implemented in order to include the attachment and detachment of influent particulate components. Nutrient uptake and oxygen release by plant roots were also simulated. This model implements fluid flow and transport equations coupled with biokinetic expressions of CWM1. It is built on COMSOL Multiphysics ^{TM} (mathematical software expensive and close source). It considers 18 components instead of 16 as in CWM1 (slowly biodegradable and inert particulate COD are divided into aqueous and solid phases) (Samo, 2014). Besides this, it includes the following processes: hydraulic sub-models for water table location, prevention of bacterial growth in dry area above the water table, solid accumulation in gravel media (Fig. 1). As described in Samso and Garcia (2013a), the schematic representation of BIO_PORE showing the inputs and outputs of the model are the following:

The governing equations of the model are discussed in Samso and Garcia (2013a). In that article, the hydraulic sub-model (using Darcy's equation), the reactive-transport sub-model (fate and transport of the aqueous phase wastewater components of CWM1 are described with reactive transport equations, one for each component, adding to reactive term accounting for the production/consumption of the substrate through microbial activity), and the biofilm sub-model and plant sub-model (the growth and decay rates of each bacteria group considered in CWM1 are described using Monod expressions) are detailed.

Samso and Garcia (2014a) introduced 'The Cartridge Theory' derived from simulation results obtained with the BIO_PORE model. The authors explained

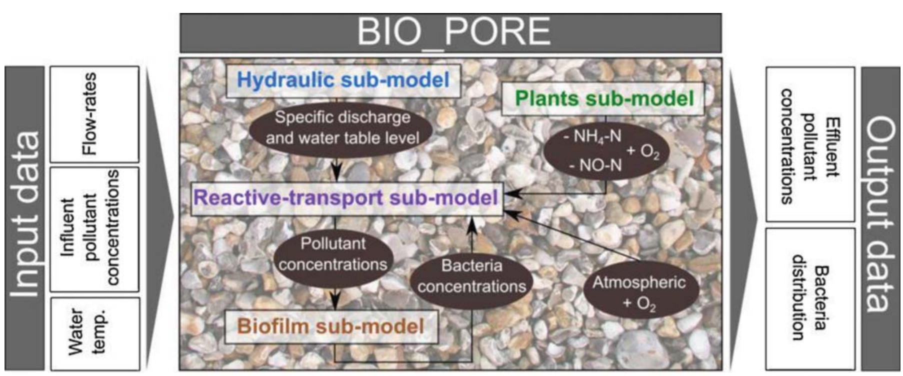

Figure 1. Schematic representation of the data flux (in the arrows) between the four sub-models (Samso and Garcia, 2013a).

the functioning of urban wastewater treatment wetlands based on the interaction between bacterial communities and the accumulated solids leading to clogging. Specifically, this theory states that the granular media of HSSF wetlands can be assimilated to a generic cartridge which is progressively consumed (clogged) with inert solids from inlet to outlet. Samso and Garcia (2013a, b) simulations revealed that bacterial communities are poorly distributed within the system and that their location is not static but changes over time, moving towards the outlet as a consequence of the progressive clogging of the granular media.

This model is in its early stage of development and is already used for simulating only a limited number of pollutants in HSSF-CWs.

3.7. CWM1 model

Langergraber et al. (2009a) introduced yet another model named CWM1 to describe biochemical transformation and degradation processes with respect to organic matter and nitrogen in both horizontal and vertical subsurface flow CWs. CWM1 describes the aerobic, anoxic, and anaerobic processes governing organic matter, nitrogen, and sulphur transformation/degradation from both soluble and particulate matter based on the ASM series (Henze et al., 2000) and the Anaerobic Digestion Model (ADM; Batstone et al., 2002).The simulated dissolved components constitute (Samso, 2014) DO, ammonia, and nitrate nitrogen (SNH and SNO), sulphate and di-hydrogen sulphide sulphur (SSO4 and SH2S), soluble fermentable COD (SF), fermentation products such as acetate (SA) and soluble inert COD (SI) and organic nitrogen as a fraction of organic matter (COD).While the particulate components include 6 functional bacterial groups, namely heterotrophic, nitrifying, fermenting, methanogenic, sulphate reducing, and sulphide oxidizing bacteria (XH, XA, XFB, XAMB, XASRB, and XSOB, respectively) and two particulate fractions of COD (XI and XS).

Rousseau et al. (2009) and Llorens et al. (2009) assessed the application potential of the CWM1 biokinetic model for simulating carbon, nitrogen, and sulphur cycles, in batch-operated conditions, through a lab-scale treatment wetland and a horizontal flow CW, respectively, to show good agreement with the measured data. Rizzo et al. (2014) also explored the capability of the HYDRUS Wetland Module to model the response of HFCW to unsteady load and included ammonium adsorption using a Langmuir isotherm in the biokinetic processes of the CWM1. Successful qualitative comparisons were also carried out between simulated and measured effluent concentrations of COD and NH_4-N by calculating the mean percentage error. In fact, Mburu et al. (2013) strongly recommends the use of CWM1 for operational CW technology development. However presently other wetland processes such as water flow in the porous media, influence of plants, transport of particles/suspended matter leading to enumeration of clogging, adsorption and desorption processes, and physical re-aeration have not as yet been considered in this model. Besides, this model is costly and requires a long computing time.

In fact CWM1 has been implemented in following different simulation platforms (Llorens et al., 2011a; Langergraber and Simunek, 2012; Mburu et al., 2012, 2013; Samso and Garcia, 2013a, b) and the resulting codes have been used to match experimentally measured effluent pollutant concentrations. Additionally, Langergraber and Simunek (2012) presented a new version of the wetland module for HYDRUS-2D that offers the possibility to choose between the already implemented CW2D and the newly implemented CWM1 biokinetic models (HYDRUS-2D-CWM1). The results showed that the two biokinetic models were implemented correctly in HYDRUS-2D.

3.7.1. CWM1-BIOPORE model

In order to take care of some of the aforementioned shortcomings of the CWM1 biokinetic model, Samso and Garcia (2013a) developed a model within the BIOPORE software framework to account for the attachment and detachment of influent particulate components (through a biofilm module) and to include nutrient uptake and oxygen release by plant roots (through a plant module). The final CWM1-BIOPORE model also includes a hydraulic module (based on the Darcy's equation) for water table location and a reactive-transport sub-model, based on the Monod equations used in CWM1, for simulating production/consumption of the substrate through microbial activity, prevention of bacterial growth in the dry area above water table, solid accumulation in gravel media, and transport of aqueous phase wastewater components in CWs.

The model is in its early stage of development and has so far been used for simulating only a limited number of pollutants in HSSF-CWs (Samso and Garcia, 2013a, b). These investigations have revealed that bacterial communities are poorly distributed within the system and that their location is not static but changes over time, moving towards the outlet as a consequence of the progressive clogging of the granular media. Based on these findings, Samso and Garcia (2014a) introduced 'The Cartridge Theory', thereby analogizing the granular media of HSSF wetlands as a generic cartridge which is progressively consumed (clogged) with inert solids from inlet to outlet.

3.7.2. CWM1-Retraso model

The CWM1-Retraso is a 2D model (Llorens et al., 2011a, b) developed using the RetrasoCodeBright software (Mburu, 2013), also called the RCB flow model, for simulating organic matter, nitrogen, and sulphur transformation processes (Ojeda et al., 2008), implemented through CWM1, and for simulating hydraulics and the hydrodynamic behaviour (Saaltink et al., 2004) of HSSF-CWs. It simulates the reactive transport of inorganic (dissolved and gaseous) species under non-isothermal saturated and unsaturated conditions, based on Darcy's and Fick's laws, using the finite-element modelling approach (Samso, 2014) and also simulates other processes viz., physical oxygen transfer, oxygen leaking from macrophytes, plant uptake, biofilm development, and media clogging. Testing and validation of the model by the authors revealed that the CWM1–Retraso model is a potential tool for investigating the hydraulics, reactive transport, and biochemical transformation/degradation of organic matter, nitrogen, and sulphur in HSSF-CWs.

3.7.3. AQUASIM_CWM1 model

AQUASIM_CWM1 is a mathematical biofilm reactor model based on the structure of CWM1 coupled to a 1D-AQUASIM's biofilm reactor compartment (Mburu et al., 2012, 2014). According to Mburu et al. (2014), the biofilm is divided into a liquid phase, consisting of 80% water in which the dissolved substances are transported by diffusion, and a solid matrix (20%) consisting of particulate components such as active and inactive bacteria and their extracellular polymeric substances.

The hybrid model has been successfully used for simulating the transformation and degradation of organic matter, nitrogen, and sulphur in CWs; and for estimating the temporal microbial growth profile and biofilm thickness in a subsurface CW. The CWM1–Aquasim–Biofilm model has also been suggested as a useful tool for analysing the influence of rhizospheric configurations on the performance of the CWs (Mburu et al., 2014).

3.8. WANG–SCHOLZ model

The Wang–Scholz 1D model (Sani et al., 2013), initially developed to simulate the evolution of liquid–solid mixture, diffusion process, and sedimentation/adsorption, basically simulates vertical flow wetland systems where clogging is considered to be a potential problem (Meyer et al., 2015). The entire process of SS sedimentation/accumulation in CWs comprises of three major mechanisms viz., settling/deposition; aggregation via coagulation; and mass exchange between SS and the dissolved phase.

The aggregation sub-model is expressed through the following governing equations:

$$\frac{\partial \emptyset i}{\partial t} = D\frac{\partial^2 \emptyset i}{\partial z^2} - (u - vi)\frac{\partial \emptyset i}{\partial z} \pm \psi i + \frac{q(z)}{A}\emptyset i, in \tag{20}$$

Where, $\emptyset i$ is the concentration of SS with particle sizes of range *i*, *t* is the time in days (d), *D* is the dispersion coefficient, *z* is the vertical elevation position (m), *u* is the vertically flowing water velocity (positive upwards, in md^{-1}), *vi*(in md^{-1}) is the fall or settling velocity of the SSs of particle size *i*, ψi is the source/sink term of the SSs of particle size *i*, $q(z)$ is the lateral inflow into the wetland (in m^3d^{-1}), A *(in* m^2*)*is the wetland area, and $\emptyset i$ is the concentration of the SS of size *i* in the lateral flow.

The mass conservation model on the other hand is expressed as:

$$\frac{\partial\emptyset}{\partial t} = D\frac{\partial^2\emptyset}{\partial z^2} - (u - v)\frac{\partial\emptyset}{\partial z} + R \tag{21}$$

Where, $\emptyset$ is the concentration of SS particles of all sizes within the treated wastewater, t is time, D is the dispersion coefficient (m), z (in m) is the vertical elevation position, u is the vertically flowing water velocity (positive upwards, in md^{-1}), v (in md^{-1}) is the fall or settling velocity of the SS, and R is the source/sink term of SS particles due to the physical adsorption on the surface of the pebbles within the CW bed.

The dispersion coefficient is expressed as:

$$Dmd = \propto u \tag{22}$$

Where, Dmd is the mechanical dispersion (m), α is the dispersivity (m), and u is the velocity (in md^{-1}) of the flowing solution, which, for continuous flow, may be estimated using Darcy's law.

Al-Isawi et al. (2014) used the Wang–Scholz Model to compare the impact of four different vertical CWs and the operational variables on their treatment efficiency and clogging processes and to model SS accumulation in the saturated zone of the system. Their results showed that serious clogging phenomena, impacting negatively on the treatment performance and the hydraulic conductivity, were not observed. The authors concluded that the performance of the Wang–Scholz Model is good for less complex operations.

3.9. Diph_M model

Petitjean et al. (2013) introduced a 1-D multiphase model for simulating multicomponent transfer in Vertcal Flow Constructed Wetland (VFCWs) based on a two-phase flow and transport module. The reactive transport module (Meyer et al., 2015) computes dissolved and gaseous oxygen concentrations and the transport of solutes such as ammonium and readily biodegradable COD. The consumption of components is governed by Monod-type kinetics based on the CWM1. Heterotrophic and autotrophic bacteria, which are responsible for COD and ammonium degradation, are also a part of the model components.

3.10. Dual-porosity model

The 1-D dual-porosity model, implemented in a HYDRUS-1D software, on the other hand, is capable of simulating preferential flow in gravel filters (Mornnavou et al., 2013a, b) under variably saturated conditions. The model assumes that the water is divided into a mobile (i.e., macroscopic pore water) and an immobile phase (constituting capillary water and water contained in the organic matter matrix). The flow was assumed to take place in only mobile phase while all exchanges were assumed to take place in both mobile and immobile phases. Water flow and solute transport were simulated using two different modelling approaches viz., the dual-porosity (non-equilibrium) model and a general equilibrium model, and the simulation data were successfully fitted to a tracer test experiment carried out on a French first-stage VFCW (Meyer et al., 2015, Mornnavou et al., 2014).

3.11. Object-oriented programming systems

Wang and Mitsch (2000), Ahn and Mitsch (2002a) and Ouyang et al. (2010) applied an object-oriented programming language-based STELLA software (Structural Thinking Experimental Learning Laboratory with Animation) for simulating wetland dynamics and the effect of biomass growth on the hydraulic properties of the saturated porous media, and for explaining the adsorption/desorption/transformation and plant uptake of pollutants. The approach has been used for a limited number of organic/nutrient pollutants and for simulating cadmium removal process in free water surface CWs (Pimpan and Jindal, 2009; Bullen et al., 2011) to reveal good fit between the observed and predicted cadmium concentrations with average cadmium removal efficiencies ranging between 61.7 and 99.6% and 74.6 and 96.5%, respectively.

3.12. RTD/GPS-X model

Samso et al. (2014b) stated that the RTD/GPS-X model is a TIS model with recycle and dead volumes under variable water contents, including COD, N (only soluble), and interaction with biofilm growth. This model combines hydraulic and kinetic modelling on fixed-bed aerated biofilm reactors. Its hydraulic model is based on Residence Time Distribution analysis (tracer injection and detection) carried out in different steps of biofilm development in the reactor. Zeng et al. (2013) showed that a hydraulic model can be chosen (PF, TIS, and TIS with exchange) depending on the shape of the breakthrough curves, regarding saturation conditions and biofilm development.

3.13. RSF_SIM model

In Germany, the RSFs were developed for assessing and monitoring the performance of CWs for combined sewer overflow treatment (CSO-CWs) (Ditmer et al., 2005). The model development combined fundamental research knowledge and lessons learnt from the application of HYDRUS-2D/CW2D (Dittmer et al., 2005; Palfy and Langergraber, 2014). Meyer et al. (2015) stated that RSF_Sim operates with a series of three stirred vertical tanks used respectively as: the retention layer (water storage), followed by the process layer (sand/gravel layer in which treatment occurs), and the drainage layer (the volume balances or water reservoir under permanent saturation).

4. Discussion

In the subject of CW modelling, many studies have been published. One can observe that the various classifications of models differ from one author to another (Rousseau et al., 2004; Langergraber, 2008, Garcia et al., 2010; Meyer et al., 2015). Kumar and Zhao (2011) classified the different modelling approaches into two broad categories: black box and process-based models. For these authors, first-order kinetic models belong to the black box category. Nevertheless, Rousseau et al. (2004) stated that these models can be classified as: regression equations, first-order model, monod-model, and mechanistic models (process-based models).

4.1. Black box models

Toscano et al. (2009) stated that CWs are widely considered as 'black boxes' due to different processes involved in pollutant removal as the results of interactions between the components of the system (soil, vegetation, water, and microorganisms) are not well known. Black box models have been used in many studies to design and predict the removal efficiency of CWs based on inputs, without capturing the internal processes governing the treatment processes. Many authors have reported satisfactory results from the use of these models but pointed out some incompleteness related to their common features. Generally, very limited types of pollutants (organics and nutrients) were tested using these models. Garcia et al. (2010) revealed that among black box approaches, the most widely used is the first-order model that is particularly suitable for sizing the systems. The weaknesses of the first-order models as described by several authors are listed as follows:

1. Kadlec (2000) showed that the parameters such as rate constants and apparent background concentrations were found to vary as a function of hydraulic loading and inlet concentration, and this variability renders the models incapable of acceptable performance with regard to design. Thus, this approach had been presented to be unsuitable to model unpredictable events, fluctuation in input flows and input concentrations, or changes in internal storages.
2. Kadlec (2000) showed numerous inadequacies in models based on first-order kinetics. The equations are based on the assumptions of prevailing PF and stationary conditions. However, small-scale wastewater treatment plants, which include most subsurface flow (SSF) CWs, often exhibit substantial influent variations and are therefore under non-steady-state conditions. Physical dispersion, short-circuiting, and dead zones are also common in SSF CWs and cause non-ideal PF conditions, which renders the first-order model unsuitable to explain satisfactorily the main nitrogen transformation processes in CWs.
3. Moreover, USEPA (2000) assumed the initial concentration to be constant in first-order model while Uddameri (2009) indicated that it may show spatial variability.

The particular features and limitations of each black box model are shown in the Table 3.

Most of the black box models have been used in many previous researches for simulating a very limited number of pollutants such as organics and nutrients and only limited types of CWs. Owing to the fact that black box models are still important despite their limitations and are used to simulate single components in process-based models (TIS, TIS with exchange used in RTD/GPS-X model; Monod equations in FITOVERT, Monod kinetics in AMS), the application of this modelling approach should be extended to the wide range of existing pollutants and to different available types of CWs.

4.2. Process-based models

Langergraber (2008, 2011) reviewed the existing mechanistic models for CWs and classified them into the following groups:

Table 3. Comparison of black-box models for CWs, their main features and limitations.

N0	Models	Main characteristics	Limitations	Reference
1	Regression models	Deals with empirical analysis of relationships between inlet and outlet concentrations from the wetlands.	Focussed on input/output data rather than on internal process data; Oversimplification; Lumped site -specific approach	Rousseau et al. (2004), Tang et al. (2009)
2	First-order models	Non-linear deterministic approach	Unable to model unpredictable events, fluctuation in input flows and concentrations, or changes in internal storages	Kadlec (2000); Kadlec and Wallace (2009); Rousseau et al. (2004)
3	Monod models	Represents first-order rate reactions for relatively low concentrations but zero-order rate reactions for high concentrations.	Prevents total decomposition of pollutants (low reaction rate for low concentrations)	Langergraber and Simunek (2005)
4	Time-dependant retardation model	Simulated removal rates decrease during a time reference; easily biodegradable substances are removed first and faster. Solution leaved with less biodegradable constituents with slower removal kinetics; more consistent parameters for COD removal data across different depths and at different loading in CWs	Requires tracer studies for computing these removal rate constants	Shepherd et al. (2001)
5	Tank-In-Series (TIS) model	Characterize the movement of pollutant as it traverses through the wetland and its discharge at the outlet, Extreme sensitivity of high levels of pollutant reduction to the character of the DTD (detention time distribution).	Focussed on I/O data rather than on internal process data	Kadlec (2003)
6	Neural Networks (ANN)	Simulates the structure and/or functional aspects of biological neural networks, simulates the removal of phenol from olive mill wastewater	Low regression coefficient for NH_3 removal	Nayak et al. (2006), Akratos et al. (2009a), Arda Yalcuk (2013)

1. Models describing the hydraulic behaviour and single-solute transport in constructed wetlands
2. Reactive transport models for saturated conditions

These categories couple reactive transport models and ideal reactor models such as series of CSTRs and/or PF reactors, respectively. In these reactors, either first-order decay rates or monod kinetics are applied to model the degradation processes of organic matter and/or nitrogen.

3. Reactive transport models for variably saturated conditions

These models include the multicomponent reactive transport module CW2D describing the biochemical transformation and degradation processes in SSF CWs. It was incorporated into the HYDRUS variably saturated water flow and solute transport program to solve additionally the Richards equation for saturated–unsaturated water flow and the convection–dispersion equation for heat and solute transport (Langergraber, 2008).

Despite the ability of these process-based models to simulate the internal processes of CWs, they present different features and limitations listed in the Table 4.

According to Meyer et al. (2015), modelling approaches can range from a simple regression to a partial differential equation model. From the comparison of the existing process-based CW models reviewed, they classified the the models into three groups according to their limitations and the field of application:

1. *Group 1* is placed for models like CWM1 and CW2D which are implemented in HYDRUS and BIO_PORE as well as for those mechanistic models using biokinetic models built on ASMs (biological transformation, degradation processes and microbial dynamics). These models were developed in subsurface flow CWs, and CWM1 and CW2D are implemented using the HYDRUS software (Langergraber and Simunek, 2011). In this group, Samso and Garcia (2013a) showed a modified version of CWM1 implemented with the COMSOL Multiphysics^{TM} platform for the BIO_PORE model.
2. *Group 2*: Process-dedicated models which offer an improved understanding of the basic science in wetland system. This category contains: Wang–Scholz Model, Diph_M, P-hydroslag model, and dual-porosity model (DPM).
3. *Group 3*: Design support models including RTD/GPS-X and RSF_Sim models.

4.3. Comparison of process-based models according to their use and availability

The process-based models listed in this study are either commercially available or free of charge. Some are accessible and not commercially available at all. Table 5 provides some supplemental comparison of the listed models according to their implementation, their simulation platform, their application, and their availability.

In recent studies, mechanistic models were shown to be important tools for describing different processes and interactions that take place within the wetland system (Garcia et al., 2010; Langergraber, 2008, 2011). In contrast, it has been

Table 4. Comparison of process-based models for CWs in their main features and limitations.

N0	Software/models	Main characteristics	Limitations	Main references
1	FITOVERT (Sotftware)	Can simulate hydraulic behaviour of VSSF-CWs in both saturated and unsaturated conditions and carbon and nitrogen transformation processes based on ASM; Software used – Matlab	Not applicable for simulating biological changes in the system.	Brovelli et al. (2007), Giraldi et al. (2010)
2	Activated Sludge Model (ASM)	Dynamic simulation of biological COD, N and P removal based on Monod kinetics	Site specific and applicable only within the conditions for which developed	Henze et al. (2000)
3	Constructed wetland Two-Dimensional (CW2D) model	Developed for vertical subsurface flow constructed wetland. CW2D 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.	Consider only dissolved substances -	Langergraber (2001) Langergraber and Šimunek (2005)
4	PHREEQC (Software)	Saturated conditions, 4 inorganic reactions, full water chemistry and water-sediment interactions	Post treatment, no biochemical model	Claveau-Mallet et al. 2012, 2014
5	PHWAT (Software)	Numerical models for simulating pH variations and clogging processes, bacteria attachement and flow-induced biofilm detachment, redox and surface complexation reactions associated with nutrients and organic pollutants based on ASMs, coupled with GW flow model MODFLOW (variably saturated conditions)	Primarily used for simulating the effect of biomass growth on the hydraulic and hydrodynamic properties of saturated porous media	Brovelli et al. (2007, 2009a, b), Mao et al. (2006), Samo et al. (2014b)
6	CWM1(Constructed Wetland Model No.1)	Degradation processes for organic matter, nitrogen and sulphur in subsurface flow CWs accounted for through simulation of porous media hydrodynamics, influence of plants, transport of particles/suspended matter, adsorption/desorption processes and physical re-aeration in constructed wetlands; uses HYDRUS wetland/2D/3D model.	Costly and long computing time	Langergraber et al. (2009a)
7	2 D HYDRUS/CWM1 (HYDRUS Software Module)	Saturated and unsaturated conditions associate to Heat transfer and root effects, removal of COD, N and S, ammonium adsorption-Platform used for simulation: HYDRUS-2D	Used for a limited number of organic/nutrient pollutants	Palfy and Langergraber, 2014 Rizzo et al. 2014

(*Continued on next page*)

Table 4. (Continued)

N0	Software/models	Main characteristics	Limitations	Main references
8	HYDRUS/CW2D -PC (HYDRUS Software Module)	Simulates carbon, nitrogen and phosphorous and forms of COD, ammonium adsorption, transformation processes (9) based on the ASM, in saturated and unsaturated conditions (Richards equations.). developed for vertical subsurface flow constructed wetland	Consider only dissolved substances - HYDRUS/ CW2D is unable to simulate COD and BOD_5 removal in periods (anaerobic processes are not modelled) and unsuitable for clogging processes	Langergraber and Simunek (2005, 2013), Langergraber, 2013 Morvannou et al. 2013, Garcia et al. (2010)
9	BIO_PORE (Software)	Saturated conditions associate to root effects, removal of COD, N and S.	Used for a limited number of organic/nutrient pollutants	Samso and García, (2013a, b)
10	Retraso Code Bright (RCB) flow model	Simulation of organic matter, nitrogen and sulphur transformation processes.	—	Ojeda et al. (2009)
11	STELLA(Structural Thinking Experimental Learning Laboratory with Animation) (Software)	Uses graphical programming language for simulating system dynamics, explaining adsorption, desorption, transformation and plant uptake of pollutants and simulating effect of biomass growth on the hydraulic properties of saturated porous media.	Used for a limited number of organic/nutrient pollutants	Wang and Mitsch (2000), Ahn and Mitsch (2002a), Ouyang et al. (2010)
12	Wang-Scholz-Model (COMSOL)	Vertical-flow wetlands with uniform Water flow, clogging process	No biochemical model	Sani et al. 2013
13	1 D-Diph_M (MATLAB)	Unsaturated (two-phase flow), forms of COD, NH4-N, oxygen		Petitjean et al. 2012 Forquet et al. 2009a, b
14	AQUASIM-CWM1 (AQUASIM Software)	Saturated conditions, simulation of organics and nutrients and S in SSF CWs, re-aeration, adsorption/ desorption COD and ammonium, plant uptake	The growth rate of bacteria are limited only by the substrates	Llorens et al. (2011a, b)
15	Dual-porosity model (DPM) in HYDRUS-1D	Variably saturated conditions	Applicable only for non-reactive tracer transport	Morvannou et al. 2013a, b
16	CMW1-RETRASO model	Number of reactions: 19 instead of 17 as in CWM1. processes included: physical oxygen transfer, oxygen leaking from macrophytes, plant uptake, biofilm development and clogging	Bacteria growth not included in the system	Langergraber et al. 2009a
17	RTD/GPS-X model	Tanks in series, under variable water content, removal of COD, N (only soluble), 11 Interaction with biofilm growth, two-step model coupling hydraulic and kinetic modelling on fixed bed aerated biofilm reactors. relies on the ASM1 model for biokinetic	Tested for very limited pollutants	Zeng et al. 2013a

(Continued on next page)

Table 4. (Continued)

N0	Software/models	Main characteristics	Limitations	Main references
		reactions. It is based on Residence Time Distribution analysis (tracer injection and detection) carried out on different steps of biofilm development in the reactor		
18	RSF_Sim	Retention Soil Filters, based on experiences in the application of HYDRUS-2D/CW2D. RSF_Sim works with three complete stirred tanks in vertical series (retention layer provides the water storage on top of the process layer, the process layer describes the sand/gravel layer as saturated during feeding, drained afterwards, in which treatment occurs, and the drainage layer improves the volume balances	Hydraulics and hydrodynamic simulations	Dittmer et al. (2005), Henrichs et al. (2007, 2009), Meyer at al. (2006), Palfy and Langergraber (2014), Meyer et al. (2013)

observed that none of these models was capable to capture all the physical, biological, chemical, and complex and delicate interactions that occur in the removal processes of pollutants in CWs (Garcia et al., 2010).

Although different types of models were reviewed and the mechanistic modelling approach was postulated as the best alternative that highlights the functionalities of CWs, various limitations were additionally observed:

1. Very few models for simulating pollutant dynamics in VSSF CWs capable of capturing the wide range of complex processes and interactions involved in the treatment process;
2. Existing models were developed for only assessing nutrients and organic pollutants in CWs;
3. Very limited efforts on modelling heavy metal dynamics in CWs;
4. Many models described are at their first stage of development and are not yet tested in different conditions and in different places worldwide.

4.4. Future considerations for modelling design and application in constructed wetlands

Considering the description and application of different modelling approaches described in this study, the constraints observed should be considered to improve the application of models in CW design and applications.

1. Formulation of models for simulating pollutant dynamics in VSSF CWs capable of capturing the wide range of complex processes and interactions involved in the treatment process;

Table 5. Comparison of process-based models according to their use and availability.

No.	Model	Biokinetic model	Dimension	Graphical user Interface for CW Modelling	CW	Pollution removal	Saturation conditions	Commercially available/Free charge	Simulation platform	Authors
1	FITOVERT (Software)	Their own	1 D	Yes	VSSF	OM, N	Variably	No	MATLAB®	Giraldi et al. (2010)
2	Activated Sludge Model (ASM)	ASM	1, 2 and 3D	/	VF/HF	OM, N, P			—	Henze et al. (2000)
3	Constructed wetland Two-Dimensional (CW2D) model	ASM	2D	/	VF	OM, N, P, O2 dissoud,	/			
4	PHREEQC (Software)	/	1D	/	VF	OM and nutrients	Saturated	Not commercially available	PHREEQC	Claveau-Mallet et al. (2014)
5	PHWAT (Software)	CW2D	1D, 2D and 3D	Hydrodynamics	VSSF	pH, redox, complexation of nutrients and OM		For Non commercialuses	PHWAT	Brovelli et al. (2009a, b)
6	CWM1(Constructed Wetland Model No.1)	ASM		/	VF/HF	OM, N, P, S	saturated	Yes, not free access		Langegraber et al. (2009a)
7	2 D HYDRUS/CWM1	CWM1	2D	Yes	HF/VF	OM, N, P, S	Variably	Yes, not open access	HYDRUS-2D	Langegraber and Simunek (2012), Pafly and Langegraber (2013)
8	HYDRUS/CW2D - PC	CW2D	2D	Yes	VF	OM, N, P, S	Variably	Yes, not open access	HYDRUS-2D	Toscano et al. (2009); Langegraber and Simunek (2012)
9	BIO_PORE (COMSOL Multiphysics)	CWM1	2D	No	HF	OM, SS, P, N, S	Saturated with variable water table	Not commercially available, not free of charge	COMSOL Multiphysics™	Samso and Garcia (2013a, b)

10	Retraso Code Bright (RCB) flow model	/	1,2 and 3D	No	HF/VF	water and gas heat or solute transport, aqueous complexation, precipitation and dissolution of minerals, sorption, and gas-liquid interaction	Variably saturated	Free of charge, source code not available	/	Saaltink et al. (2004)
11	STELLA (Software)	/	Dynamic	Yes	HF/VF	OM, N,P, metals	/	Yes, not free of charge	/	Ouyong et al. (2010)
12	Wang-Scholz-Model (COMSOL)	/	1D	No	VF	SS	Saturated	Not commercially available	COMSOL Multiphysics^{TM}	Sani et al. (2013)
13	1 D-Diph_M (MATLAB)	ASM1	1D	/	VF	OM, Gaseous fluxes estimation	Variably saturated	Open access on demand	MATLAB	
14	AQUASIM-CWM1	CWM1	0D	No	CSTR	OM, P, N, S	Saturated	Not commercially availble, free of charge	AQUASIM	Mburu et al. (2012)
15	Dual-porosity model (DPM) in HYDRUS-1D	/	1D	Yes	VF (French -type)	(Simulation of preferential flow in gravel)	Variably saturated	Commercially available	HYDRUS-1D	
16	CMW1-RETRASO model	CWM1		No	HF	OM, N, P, S	Saturated	Not commercially available, free of charge	RetrasoCodeBright (RCB)	Mburu et al. (2013); Liorens et al.(2011a, b, 2013)
17	RTD/GPS-X model	ASM1	/	/	Tanks in series, Plug Flow, Tanks in Series with Exchange	TOC, NH4-N	Saturated	Not commercially available	GPS-X	Zeng et al. (2013a, b)
18	RSF_Sim	Their own	1D	No	VF	COD, N,	Variably	In preparation for non commercial uses, open access for scientific purpose	MS Excel	Meyer (2011); Meyer et al. (2013), Meyer et al. (2015)

Table 6. Current criteria necessary for selecting a model according to the user's needs.

Step 1	Which model do you need for your system?		
	- Type of constructed wetland	VF/HF	
	Hydraulic and hydrodynamic		Saturated conditions saturated/unsaturated
		Feeding strategies	Cycles/continuous
		Evapotranspiration	
		Clogging	
	Biokinetic model	- Biochemical degradation a nd transformation	- Functional bacterial groups - Bacterial growth and their activities
		Biomass description	
	Physic-chemical processes	- Atmospheric oxygen transfer	Redox, pH, chemical equilibrium, particulate transport, filtration/sedimentation/sorption
		- Gas transport,	
Step 2	Which model fits your needs?	Check the design simplicity or complexity, spatial resolution (low/high), simulation (short-term/long-term)	
Step 3	Which resources are required?	User training level/price	

Source: Adapted from Meyer et al. (2015).

2. Extension of models for the assessment of not only nutrients and organic pollutants in CWs, but the wide range of pollutants found in different compartments of the environment
3. Application of different tests for different studies in different places worldwide.

4.5. Criteria of model selection

Table 6 indicates the necessity for users to consider 3 steps for selecting a model adequate for the needs of a particular CW. Indeed, the user should know the type of system and all the processes involved in the treatment process. The simplicity or the complexity of the model as well as the efficiency should be checked. Finally, the user should assess the resources required for the proper application of the model.

5. Conclusions

Although reviews are already available in the literature, this text summarizes all state-of-the-art knowledge and development in the field of modelling approaches applied in CW, the strength and weakness of each type of model, their availability and the criteria of their selection. Thus, this paper is a useful summary of the modelling status in CWs. CWs in recent decades are considered by several authors as an effective alternative to conventional systems for the treatment of agricultural, industrial, and municipal wastewater. Numerous models have been developed for simulating and predicting the behaviour of CWs over an extended period of time. These are categorized as black box and process-based models. In the black box category the first-order model is still widely used to design CWs but has numerous inadequacies with regard to predicting the outlet contaminant concentrations.

Despite the fact that mechanistic models highlight the comprehension of internal processes involved in pollutant dynamics in CWs, they are still unable to take into account all the processes and interactions that exist in CWs. Besides this, more studies should be devoted to modelling heavy metal dynamics in CWs and especially more modelling studies should be extended to SSF CWs and hybrid systems for improving their performances in effective wastewater treatment processes.

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