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# 1 A review on numerous modeling approaches for effective,

# economical and ecological treatment wetlands

4 J.L.G. Kumar, Y.Q. Zhao\*

- 6 Centre for Water Resources Research, School of Architecture, Landscape and Civil
- 7 Engineering, University College Dublin, Newstead, Belfield, Dublin 4, Ireland

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9 (\* Corresponding author: Y.Q. Zhao; E-mail: yaqian.zhao@ucd.ie)

#### ABSTRACT

Constructed wetlands (CWs) for wastewater treatment have evolved substantially over the last decades and have been recognized as an effective means of "green technology" for wastewater treatment. This paper reviews the numerous modeling approaches ranging from simple first-order models to more complex dynamic models of treatment behaviour in CWs. The main objective of the modeling work is to better understand the process in CWs and optimize design criteria. A brief study in this review discusses the efforts taken to describe the process based model for the efficient removal of pollutants in CWs. Obtaining better insights is essential to understand the hydraulic and biochemical processes in CWs. Currently, employed modeling approaches can be seen in two categories, i.e. "black-box models" and "process-based models". It is evident that future development in wetland technology will depend on improved scientific knowledge of internal treatment mechanisms.

24 Keywords: Constructed wetlands, Reed bed, Rate constant, Kinetics, Black-box model, 25 Process-based model. 26 27 1. Introduction 28 2. Current status of CW models 29 2.1Black-box models category 30 2.1.1 Regression models 31 First-order models 2.1.2 32 Time dependent retardation model 2.1.3 33 2.1.4 Tank-in-series model 2.1.5 34 Monod model 35 2.1.6 Neural Networks 36 2.1.7 Statistical approaches 37 2.2 Process-based model category 38 2.2.1 FITOVERT model 39 2.2.2 CW2D model 40 2.2.3 STELLA Software 2.2.4 PHWAT Software 41 42 2D mechanistic model 2.2.5 43 2.2.6 CWM1 44 3. Discussion 45 3.1 Black-box models 46 3.2 Process-based models 47 4. Summary and conclusions

#### 1. Introduction

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Industrialization, urbanization and inadequate disposal practices precede a mammoth pollution problem in water environment including rivers, estuaries, lakes and oceans (Zhao et al. 2009). One of the sustainable wastewater treatment alternatives is the implementation of CWs since they are efficient, low-cost, easy to use and eco-friendly (Naz et al. 2009). Compared with natural wetlands which have large variability in functional components and thus unknown and unstable treatment capability, CWs can be built with a much higher degree of control, thus allowing the establishment of experimental treatment facilities with a well-defined composition of substrate, type of vegetation and flow pattern. As such, CWs are often termed as "engineered wetlands" (Knight et al. 1999; Haberl et al. 2003; Babatunde et al. 2009). Pollutants in CWs are removed through a combination of physical, chemical, and biological processes including sedimentation, precipitation, adsorption, assimilation by the plant tissue and microbial transformations. The main advantages of using CWs are flexibility in sizing and site selection, control over hydraulic pathways and retention time. In addition to this, CWs are well recognized as having low construction and maintenance cost and low energy requirement. However, it has to be noted that CWs are a land intensive treatment option and show in some extend a stochastic behavior (Haberl et al. 2003).

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Treatment behaviour in CWs is often considered to be figurative black-box (Rousseau et al. 2004). Detailed understanding of CW functioning is still desirable because a large number of physical, chemical and biological processes occur in parallel and influence each other. Until now, CWs design has been mainly based on rules of thumb approaches using specific surface area of requirements (Brix and Johansen, 2004) or simple first-order decay

72 models (Kadlec and Knight, 1996; Rousseau et al. 2004). The increasing application of 73 CWs for wastewater treatment and strict water quality standards is an ever growing 74 incentive for the development of better process design tools (Rousseau et al. 2004). 75 Originally, working with simple regression equations, most researchers and designers evolved towards the use of the well known first-order k-C\* model (Kadlec and Knight, 76 77 1996). However this black-box model is based on only two parameters, the first-order 78 decay rate k, and the background concentration, C\*, which is an obvious over 79 simplification of the complex wetland processes. As has been indicated by Kadlec (2000) 80 the first-order model is inadequate for the design of treatment of wetlands. More recently, 81 several dynamic, compartmental models were developed by several researchers such as 82 Mayo and Bigambo (2005), Nabizadeh and Mesdaghinia (2006), Brasil et al. (2007) 83 Langergraber et al. (2008), Giraldi et al. (2010) and Pimpan and Jindal, (2009). These 84 studies have shown promising results for the CW processes for various wastewater 85 treatments. Therefore attentions and attempts have been made to CWs modeling and this 86 paper tries to review such developments.

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#### 2. Current status of CWs models

- 89 CW models range from simple simulation models such as empirical, numerical and
- statistical models to more complex process-based model. The details of the current status
- 91 of CWs modeling is presented below.

#### 2.1 Black-box model category

- 93 2.1.1 Regression models
- 94 Majorities of the investigations on treatment wetlands have mainly been focussed on
- 95 input-output (I/O) data rather than on internal process data. An empirical regression

analysis is often performed to determine if significant relationships existed between inlet and outlet concentrations of the wetlands. As a whole, regression equations seem to be the useful tools in interpreting and applying these I/O data (Rousseau et al. 2004). Stone et al. (2002) used the regression equation (Eq. (1)) to predict the outlet concentration in swine lagoon wastewater treatment.

$$C_{out} = aC_{in}^b q^c \tag{1}$$

Where,  $C_{in}$  is inlet concentration,  $C_{out}$  is outlet concentration, q is the hydraulic loading rate HLR (m d<sup>-1</sup>), a, b, c is regression coefficients. With the help of a regression analysis, Tang et al. (2009) successfully employed multivariate linear regression equations for effluent benzene prediction in a study of benzene removal in vertical-flow CWs. Effluent benzene is set as a function of effluent dissolved oxygen, electric conductivity, redox potential, pH and temperature of the wetland system. Though the regression equations provide useful information on the overall performance of the wetlands, they are typically valid only for the range of data used to model them. It has been mentioned that although the literature values focus on the wide range of variety of the wetland systems, cautions should be paid to compare the empirical regression equations since they were derived from large varieties of wetland scales, wastewater strength (Stone et al. 2002), environmental conditions and species of cultivated plants.

114 2.1.2 First-order models

Many individual wetland processes are basically first-order, such as mass transport, volatilization, sedimentation and sorption (Kadlec and Wallace, 2009). First order models are used commonly for the design of treatment wetlands using either Eq. (2) or Eq. (3)

$$118 \qquad \frac{C_{out}}{C_{in}} = e^{\frac{k_A}{q}} \tag{2}$$

where  $k_A$  is the areal decomposition constant (m d<sup>-1</sup>)

$$\frac{C_{out}}{C_{in}} = e^{-k_v t} \tag{3}$$

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where t is HRT in days,  $k_v$  is the volumetric decomposition constant (m d<sup>-1</sup>). Several authors including Kadlec et al. (2000), Knight et al. (2000), Stone et al. (2004), Sun et al. (2005), Jamieson et al. (2007) and Stein et al. (2007) have published papers relating to the first-order model application in CWs. This approach has been used for design and to predict almost all major pollutants such as organic matter (OM), suspended solids (SS), nitrogen (N) and RP (Mitchell et al. 2001). Jamieson et al. (2007) reported that the efficiency of treated livestock wastewater in cold climates was found reasonably well but the performance is poor in regard to P removal. The size of the wetland was kept at approximately 5m wide and 20m long, consists of deep zones and shallow zones which are vegetated with cattails (Typha Latifolia) and duckweed (Lemna spp). The corresponding  $k_A$  for water quality parameters is 0.026 m d<sup>-1</sup> for biological oxygen demand (BOD<sub>5</sub>), 0.011 m d<sup>-1</sup> for total phosphorus (TP), 0.018 m d<sup>-1</sup> for total Kjeldahl nitrogen (TKN), 0.019 m d<sup>-1</sup> for ammonium nitrogen (NH<sub>4</sub><sup>+</sup>-N), 0.005 m d<sup>-1</sup> for ammonia nitrogen (NO<sub>3</sub>-N) and 0.023 m d<sup>-1</sup> for total suspended solids (TSS). Interestingly, after adjusting the outlet concentration for dilution the rate constant values were lowered by at least 0.005 m d-1 compared with the  $k_A$  values reported by Reed et al. (1995) and Kadlec and Knight, (1996). Stone et al. (2004) reported the much lower  $k_A$  values for the marsh-pond-marsh wetland systems. However it is justified that the low reaction rate constant is due to higher hydraulic loading in the system. Kadlec (2000) pointed out that the inadequacies of firstorder model are due to the variability caused by unpredictable events such as fluctuation in input flows and concentration and henceforth changes in internal storages, as well as by weather, animal activity and other ecosystem factors. However, the first-order model is still considered as an appropriate design equation for pollutant removal in CWs (Kadlec and Wallace, 2009). Rousseau et al. (2004) gave a comprehensive and critical review of first-order rate constants for horizontal subsurface flow (HSSF) constructed treatment wetlands. These are commendable efforts to address the reaction rates taking place in the treatment wetlands and help the designer to harmonize design guidelines. Although first-order model looks simple, it represents the highest level of complexity that can generally be calibrated with wetland data and provides a reasonable approximation of performance for a wide range of pollutants in wetlands (Knight et al. 1999).

2.1.3 Time-dependant retardation model

Due to inadequacies in first-order model, Shepherd et al. (2001) introduced the timedependent retardation model for chemical oxygen demand (COD) removal that replaces the background concentration  $C^*$  by two other parameters  $K_0$  and b. It has been assumed that removal rates decrease during the course of time, because easily biodegradable substances are removed first and fast, thus leaving a solution with less biodegradable constituents and hence with slower removal kinetics. This continuous change in solution composition can be represented by a continuously varying volumetric first-order rate constant,  $k_{\nu}$ , as shown in Eq. (4)

161 
$$k_{v} = \frac{K_{0}}{(b\tau + 1)}$$
 (4)

Where,  $K_0$  is initial first-order volumetric rate constant (d<sup>-1</sup>), b is time based retardation coefficient (d<sup>-1</sup>) and  $\tau$  is retention time (d). This model was considered to be more appropriate for CW design because it allows a steady decrease in COD (or any other component) with increased treatment time rather than a constant residual COD, C\* value.

167 2.1.4 Tank-in-series (TIS) model

It has been evident that many treatment wetland variables and parameters do not possess single unique values but are distributed with respect to some wetland attribute (Kadlec, 2003). Water travels in wetlands through fast and slow tracks due to vegetation, topography and other environmental factors (Kadlec and Knight, 1996). This leads to distribution of detention times in wetlands. These distributions may be due to velocity profile effects and no contribution from the mixing processes (Kadlec 2003). Numerous mechanistic models have been utilized to describe wetland detention time distribution (DTD), i.e. tank-in-series (TIS), plug flow (PF) with dispersion (Kadlec and Knight, 1996). The most common model is TIS and the result is a gamma distribution with n=N and  $\beta = t_i$  as shown in Eq. (5)

178 
$$g(t) = \frac{1}{t_i(N-1)!} \left(\frac{t}{t_i}\right)^{N-1} \exp\left(-\frac{t}{t_i}\right)$$
 (5)

t is detention time (d),  $t_i$  is mean detention time in one tank (d). N is number of tanks.

TIS mixing can be described through gamma distribution but the distribution time does not suggest the turbulent mixing existence. Therefore gamma distribution can be caused from totally unmixed and separate travel paths with different velocities (Kadlec, 2003). The end result of all experiments and models is the prediction of extreme sensitivity of high levels of pollutant reduction to the character of the DTD. The number of tanks in the TIS-model represents the degree of mixing. A high value of N means a small degree of dispersion and thus the presence of a PF reactor. If N=1, then a single combined stirred tank reactor (CSTR) is defined (Kadlec and Knight, 1996; Persson and Wittgren, 2004). Uddameri (2009) used the TIS model to characterize the movement of pollutant as it traverses through the wetland and is discharged at the outlet. The below mentioned TIS (Eq. (6)) has

been suggested by to offer a better platform to accommodate distributed parameters

191 (Kadlec, 2003)

192 
$$\frac{C_{out}}{C_{in}} = \frac{1}{(1 + k_{VRC}t/N)^{N}}$$
 (6)

 $k_{VRC}$  is first order volumetric rate constant (d<sup>-1</sup>),

2.1.5 Monod models

196 The transition from first to zero-order biological degradation kinetics due to increased load

can be represented by the well-known Monod expressions, as shown in Eq. (7).

198 
$$r = k_{o,v}V \frac{C}{K_{HSC} + C}$$
 (7)

where r (mg d<sup>-1</sup>) is the rate of biological degradation and  $K_{HSC}$  (mg m<sup>-3</sup>) is the so called half-saturation constant, C is contaminant concentration (mg m<sup>-3</sup>)  $k_{0,V}$  is zeoreth-order volumetric rate constant (mg m<sup>-3</sup> d<sup>-1</sup>). When  $C << K_{HSC}$ , kinetics are first-order and as C increases, the kinetics become saturated. Monod kinetics reveals that the loading rate and the zero-order degradation rate constant are essential parameters for efficient wetland design for the removal of organic carbon in subsurface flow (SSF) CWs (Mitchell et al. 2001). Most process based models use Monod type expressions for describing the reaction rates, not only CW2D (Langergraber, 2005). One of the interesting features of this model is an alternative explanation of  $C^*$ . Indeed, if concentrations drop to near zero, the Monod equation predicts a very low reaction rate, which may prevent total decomposition of the pollutant within the given HRT. Kemp and George (1997) used a comparable model to represent ammonia removal in a pilot scale HSSF- CWs treating domestic wastewater. They found a  $k_{0,V}$  of 7.8 mg  $L^{-1}$ d<sup>-1</sup> for N and a  $K_{HSC}$  value of 5 mg  $L^{-1}$  for N. The coefficient of determination  $R^2$  indicated that the Monod type model better described the

variability of the data than a first-order model. Sun et al. (2008) used Monod and firstorder kinetics for the removal of organic matter in horizontal flow reed beds in United Kingdom and stated that the sizing of horizontal flow reed beds is primarily based on

organic matter BOD<sub>5</sub> and Kickuth equation as shown in Eq. (8), which is a combination of

217 first-order kinetics and PF model.

218 
$$A_h = Q (\ln C_{in} - \ln C_{out})/k$$
 (8)

Where,  $A_h$  is the surface area of a single horizontal flow reed bed (m<sup>2</sup>), Q is the daily flow

rate of wastewater ( $m^3 d^{-1}$ ), k is general first-order reaction rate constant ( $m d^{-1}$ ).

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222 2.1.6 Neural networks

223 An ANN (Artificial Neural Network) which is usually called "neural network" (NN), is a

224 mathematical or computational model that tries to simulate the structure and/or functional

aspects of biological neural networks. ANN is well known for forecasting/predicting,

226 pattern recognition and process control in most of the areas in science and technology

(Nayak et al. 2006). Akratos et al. (2009a, b) derived a design equation through ANN for

the removal of TN in CWs. A design equation for TN removal is proposed in their work as

an alternative to the first-order model, as shown in Eq. (9) and Eq.(10).

$$230 R_{TN} = \frac{HRT}{K_{TSRP} + HRT} (9)$$

231 with 
$$K_{TSRP} = \left(\frac{22.8}{T}\right) 45.5 \left(\frac{n}{1-n}\right)^3$$
 (10)

where  $R_{TN}$  is TN removal, HRT and  $K_{TSRP}$  is time scale of the removal process, days, n is

233 the porosity and  $\left(\frac{n}{1-n}\right)$  is an expression which includes many formulas predicting

234 hydraulic conductivity in porous media (Sidiropoulou et al. 2007). The above mentioned

hyperbolic equation combines zero and first-order kinetics as this is considered most handy for CWs. The performance of the design equation appears to be reasonably good for NH $_3$  removal despite relatively low regression coefficient  $R^2$  = 0.42. Naz et al. (2009) compared the performance of HSSF- and free water surface flow (FWSF)-CWs and modeled the performance using an ANN-back propagation algorithm. The results showed that  $R^2$  values for predicting effluent total chemical oxygen demand (TCOD), soluble chemical oxygen demand (SCOD) , and total biological oxygen demand (TBOD) of HSSF-CW were 0.90, 0.90 and 0.94, respectively, whereas the  $R^2$  values for FWSF-CW were 0.96, 0.74 and 0.84, respectively. ANN predictions may allow the process engineer to take some measures to overcome possible process upsets. Tomenko et al. (2007) compared multiple regression analysis (MRA) and two (ANN)- multilayer perceptron (MLP) and radial basis function network (RBF) for the prediction of BOD. The results revealed that MRA as well as ANN models were found to provide an efficient and robust tool in predicting CW performance.

The SOM (Self Organizing Maps) is also a neural network model and algorithm that implements a characteristic non-linear projection from the high-dimensional space of sensory or other input signals onto a low dimensional array of neurons and has been widely applied for visualization of dimensional systems and data mining (Kohonen et al.1996). Zhang et al. (2008, 2009) applied SOM to predict the outlet concentration of BOD<sub>5</sub>, NH<sub>3</sub>-N and P in the integrated constructed wetlands (ICW) treating farmyard runoff. The results revealed that the above parameters plus the temperature, conductivity and dissolved oxygen were predicted well using SOM model. SOM can also be applied to predict the heavy metal removal in CWs (Lee and Scholz, 2006). Scholz et al. (2007) have

applied the self-organizing Kohonen map as a novel modeling approach to few CWs datain Ireland.

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## 2.1.7 Statistical approaches

Stein et al. (2007) applied two statistical techniques known as Levenberg-Marquardt (L-M) method and Non-linear mixed effects (NLME) to fit the k-C\* model to data set consisting of 192 time-series COD concentrations measured from batch loaded SSF wetlands. Temperature based reaction rate constants (k<sub>20</sub>) were obtained for all the three plant species treatment; such as Carex utriculata, Schoenoplectus acutus, Typha Latifolia and control.  $k_{20}$  (d<sup>-1</sup>), calculated using L-M method for Carex utriculata was 0.896, 0.783 for Schoenoplectus acutus, 0.688 for Typha Latifolia and 0.615 for the control whereas the reaction rate constant calculated using NLME method was 0.925 for Carex utriculata, 0.743 for Schoenoplectus acutus, 0.612 for Typha Latifolia and 0.366 for the control. Therefore, it was concluded that that the magnitude of the coefficients varies strongly by species. Sun and Saeed (2009) examined the accuracy of four design approaches including Monod-kinetics, first-order kinetics, CSTR and PF patterns using three statistical parameters (coefficient of determination, relative root mean square and model efficiency) for the organic matter removal in 80 horizontal flow reed bed for domestic sewage treatment. They found that the combination of Monod kinetics and PF have good agreement with theoretical and actual performance data. However the statistical analysis approach requires a large amount of performance data from different experimental conditions which is a challenging task.

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### 2.2. Process-based model category

283 2.2.1 FITOVERT model (mathematical model for vertical subsurface flow, VSSF-CWs) 284 Relatively few numerical models specifically developed to simulate CWs have been 285 reported (Brovelli et al. 2007). Most of the currently available models can simulate HSSF-286 CWs (Giraldi et al. 2009) but only few models can simulate VSSF-CWs (Langergraber and 287 Simunek, 2005). To bridge the gap in VSSF-CWs, Giraldi et al. (2009) developed a 288 mathematical model, called FITOVERT. It can simulate the hydraulic behaviour of VSSF-289 CWs in both saturated and unsaturated conditions. Biodegradable OM and N compounds in 290 FITOVERT model was developed by using activated sludge model 1 (ASM 1) (Henze et 291 al. 2000). On the other hand, FITOVERT can also handle the porosity reduction due to 292 bacteria growth and accumulate of particulate components, so that the clogging process is 293 also simulated as an effect of pore size reduction on the hydraulic conductivity of the 294 simulated system. The relationship between pressure head, hydraulic conductivity and 295 water content was explained through Van Genuchten-Mualem functions (Van Genuchten, 296 1980) which is shown in Eq. (11).

297 
$$K_{USHC} = K_{SHC} \left( \frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{0.5} \left[ 1 - \left( 1 - \left( \frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{\frac{1}{m}} \right)^m \right]^2$$
 (11)

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where  $K_{USHC}$  (cm s<sup>-1</sup>) is the unsaturated hydraulic conductivity,  $K_{SHC}$  (cm s<sup>-1</sup>) is the saturated hydraulic conductivity,  $\theta$  is the volumetric water content,  $\theta_r$  and  $\theta_s$  are the residual and saturated hydraulic conductivity, m is the empirical parameter for unsaturated conditions. It has to be pointed out that most of the values were obtained for FITOVERT model based on an extended literature analysis. The  $K_{SHC}$  obtained from the pilot VSSF-CW for six different layers ranges from 8 to 20 cm (thickness) and the particle size (20-60 mm) and its corresponding saturated hydraulic conductivity was found between 0.169 to 2,

cm s<sup>-1</sup> The efficiency of the model was reported as 0.990 for partial saturation condition whereas 0.979 for complete saturation condition (Giraldi et al. 2009).

2.2.2 Constructed wetland two dimensional (CW2D) model

The first implemented HYDRUS-2D was used as a starting point for the CW2D implementation. However, the software is now called HYDRUS (Simunek et al., 2006, See http://www.pc-progress.com). The multi-component reactive transport model CW2D for sub-surface flow CWs was developed by Langergraber and Simunek (2005) as an extension of HYDRUS-2D variably saturated flow and solute transport package. Biochemical transformations in CW2D are based on the ASM (Henze et al. 2000). The main drawback of CW2D is that up till now only dissolved substances are considered and it is necessary to consider particulate wastewater constituents for the realistic model (Langergraber and Simunek, 2005).

Langergraber (2003) used CW2D model which consists of different layers (main, intermediate and drainage) filled with various size of the gravel planted with Arundo donax (giant reed) to focus mainly on the hydraulic behaviour of the CWs. Results reveals that the reactive transport simulations with CW2D fit the measured data well for the pilot scale CWs. Toscano et al. (2009) modeled the pollutant removal in a pilot scale two stage subsurface flow CWs. Flow and single solute transport was described using HYDRUS-2D whereas the transformation and elimination processes of organic matter and nutrients were described using multi-component reactive transport module CW2D. Simulation results fit well with the measured data of pollutant removal processes, water flow and tracer data.

329 2.2.3 STELLA (Structural Thinking Experimental Learning Laboratory with Animation)

330 Software

STELLA is a graphical programming language especially for system dynamics study. To model and better understand the non-linear dynamic systems in CWs many researchers used STELLA graphical programming language such as Wang and Mitsch (2000), Ahn and Mitsch (2002) and Ouyang et al.(2010). Pimpan and Jindal (2009) explained the adsorption, desorption and plant uptake in the laboratory scale FWSF-CWs planted with bulrush (Cyperus Corymbosus Rottb) using the STELLA software. The simulated and measured average cadmium ( $C_d$ ) removal efficiencies were in the range of 61.7- 99.6 % and 74.6 - 96.5 %, respectively. Since the measured and simulated values are in good agreement, it has been recommended to use the developed mathematical model for the  $C_d$  removal. Mayo and Bigambo (2005) studied the process of N transformation in HSSF-CWs. It has been found that the sedimentation and the regeneration mechanisms accounted for 0.872 g m<sup>-2</sup> d<sup>-1</sup> and 0.752 g m<sup>-2</sup> d<sup>-1</sup> of N transformation respectively. Significant transformations were also observed through denitrification and nitrification which were responsible for 0.436 g m<sup>-2</sup> d<sup>-1</sup> and 0.425 g m<sup>-2</sup> d<sup>-1</sup> of transformed N respectively. However N removal through plant uptake requires plant harvesting from the wetlands.

#### 2.2.4 PHWAT Software

Brovelli et al. (2009) presented a modular modelling tool suitable for simulating the clogging process in 1, 2 and 3D. A new clogging module was implemented for the numerical model which evolved from PHT3D. PHWAT is a computer code for 3D reactive transport in variable-density saturated flow. This numerical model is able to simulate the effect of biomass growth on the hydraulic properties of saturated porous

media, i.e. bioclogging. The model is developed at the macro-scale, and includes the effect of flow-induced shear stress on biofilms. This model has greater flexibility because of an arbitrary reaction network and the multiple components can induce pore clogging. The simulation results demonstrated that the rate and patterns of bioclogging development are sensitive to the initial biomass distribution.

#### 2.2.5 2D mechanistic model

Ojeda et al., (2008) used a two-dimensional (2D) mechanistic mathematical model in order to evaluate the relative contribution of different microbial reactions to organic matter removal (in terms of COD) in HSSF-CWs that treated urban wastewater. The model is based on the code RetrasoCodeBright, which has been modified to include the main microbial processes related to organic matter and nitrogen transformations in the wetlands. In their study, they also evaluate how changes in the organic loading rate affect both organic matter removal efficiency and the relative importance of the microbial reactions.

#### 2.2.6 CWM1 (Constructed Wetland Model No.1)

Langergraber et al., (2009) presented a general biokinetic model to describe biochemical transformation and degradation processes for organic matter and nitrogen in subsurface flow CWs. CWM1 considers the biokinetic processes in HF and VF CWs and the main objective is to simulate the effluent concentration. They suggested to include other processes including porous media hydrodynamics, the influence of plants, the transport of particles/suspended matter to describe clogging processes, adsorption and desorption processes and physical re-aeration must be considered for the formulation of a full model for constructed wetlands. It is believed that CWM1 such as the IWA ASMs, will become a

377 widely accepted model formulation for biochemical transformation and degradation 378 processes in subsurface flow CWs and will be implemented in many simulation platforms.

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#### 3. Discussion

381 The above listed efforts of modeling in CWs can be seen clearly in either black-box 382 models or process based models

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#### 3.1 Black-box models

- 385 It is realized that most models used in CWs were based on input/output data (Rousseau et 386 al. 2004) and the treatment processes in wetland were considered as a black-box, as 387 illustrated in Fig. 1. On the other hand PF assumption seems to be reasonable 388 approximations to the hydraulic conditions in the wetland (Kadlec, 2000). Furthermore 389 imperative issue of the background or the initial concentration in the wetland is assumed 390 to be constant in most first-order modeling efforts (USEPA, 2000). In reality, the initial 391 concentrations in the wetland may exhibit spatial variability (Uddameri, 2009). Kadlec (2000) made a distinction between true background concentration (C<sub>b</sub>) and apparent 392 background concentration (C<sub>a</sub>\*). Constants of k and C\* are in fact the function of the 393 wetland characteristics and operating conditions, as shown in Eq. (12) and Eq. (13), 394 respectively.
- 395

396 
$$k = \psi_k = (h, q, C_{i_n}, D, P - ET)$$
 (12)

397 
$$C^* = \psi_{C^*} = (h, q, C_{in}, D, P - ET)$$
 (13)

where D is the wetland dispersion coefficient (m<sup>2</sup> d<sup>-1</sup>),  $\Psi_k$  is the rate constant function 398 symbol,  $\Psi_{C^*}$  is the apparent background concentration symbol (g m<sup>-3</sup>), h is free water 399 depth (m), P is precipitation (m d<sup>-1</sup>), ET is evapo-transpiration (m d<sup>-1</sup>). 400

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## [Insert Fig.1 here]

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Interestingly, when water flows in the wetland it passes through diverse vegetation and it leads to short-circuiting which impacts on the treatment (Kadlec, 2000). In TIS model wetland is partitioned into a number of equally sized CSTRs reactor tanks and the concentration "C" of a certain pollutant leaving each tank is equal to the uniform internal concentration (Kadlec and Knight, 1996). Retardation model is considered as one of the efficient method for designing CWs because it allows a steady state decrease in COD (or any other component) (Shepherd et al. 2001). Kadlec and knight (1996) acknowledged the time-dependent nature of the BOD<sub>5</sub> (or COD) removal constant, but did not further analyze the retardation rate of the decay constant. It is worth noting that the performance of CWs normally analyzed on the basis of first-order degradation kinetics often limited by a residual outlet concentration. However, biological systems are more likely to operate under Monod-type kinetics, where degradation rates are limited by pollutant availability at relatively low pollutant concentration, and saturated at relatively high pollutant concentration (Mitchell et al. 2001). Several researchers have determined the reaction rate constant (k<sub>A</sub>, k<sub>V</sub>, k<sub>20</sub>, k<sub>0</sub>, k<sub>HSC</sub>, k<sub>TSRP</sub>, k<sub>0,V</sub>, k) for different types of CWs. Interestingly, 'k' values reported by several researchers are not the same because all the experiments have been carried out under different set-up and environmental conditions. However there is a lack of data to draw conclusions for a unique 'k' values for the removal rates. Even if CWs are widely used and studied, they are often describes as "black-boxes" where the interactions between soil vegetation, water and microorganisms are not well known (Toscano et al. 2009). This perplexing situation leads to numerical models with different complexities to better understand the process in CWs.

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Efforts at applying statistical techniques to interpret the CW data have been made in recent years (Scholz, 2003; Stein et al. 2007; Sun and Saeed, 2009). The only limitation is large number of data sets required for the application of any statistical packages. A few authors such as Tomenko et al. (2007), Akrtos et al. (2009a, b) and Naz et al. (2009) applied ANN for modeling in CWs and used for prediction purpose. Though it has been considered as a robust tool the principal drawback is that it is typically used as a "black-box" approach, hiding the internal process mechanisms. Like ANN, the other standard tool named SOM can be applied in CW modeling (Lee and Scholz, 2006; Scholz et al., 2007; Zhang et al., 2008). SOM model can also be used as a prediction tool for the daily control of wetland system. However, application of SOM models in wastewater treatment process control is relatively new (Hamed et al. 2004; Grieu et al. 2005). GIS is a powerful tool which can also be used in CWs for mapping, siting, sizing of wetlands (Trepel and Palmeri, 2002; Li and Chen, 2005; White and Fenney, 2005). The size of the watersheds, the flow processes (that drive wetland functions) and the characteristics (that influence wetland biological and biogeochemical characteristics) make it advantageous to automate these procedures using GIS (White and Fennessy, 2005).

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## 3.2 Process-based models

Process-based models allow the increased understanding of the processes occurred in the "black- box" CWs (Langergraber, 2007). These models can provide insight into the "black-box" and gives indulgent information which helps highly for the design purpose.

Results obtained from the hydraulic model of FITOVERT seem to be better for the simulation in both saturated and unsaturated conditions for the VSSF-CW, but the biochemical model has not been published yet (Giraldi et al. 2009). HYDRUS is a simulation tool in which CW2D module has been implemented to simulate transport and reactions of the major pollutants including OM, N and P in CWs (Toscano et al. 2009). It is worth noting that these process based models are highly sensitive and dependent on temperature especially for N transformations. It has been reported that by introducing temperature dependencies for half-saturation constants for the hydrolysis and nitrification processes it is possible to simulate COD and NH<sub>4</sub>-N effluent concentration at low temperatures (Langergraber, 2007). STELLA is a good example of mathematical-based software, however it is recommended that further calibration and validation of the developed model using STELLA software is still required in CWs. Brovelli et al. (2009) observed the largest degree of variability in the simulations where the initial biomass concentration was a log-normal spatially correlated random distribution. It has been concluded that the quantitative prediction of rate of bioclogging is possible only when the initial conditions are well characterized. Ojeda et al. (2008) evaluated the importance of different microbial reactions on organic matter removal in horizontal subsurface flow CW. It has been reported changing influent COD concentration (for example from 290 to 190 mg/L) while maintaining a constant HLR has a smaller impact, causing efficiency to increase from 79% to 84%. Changes in influent COD concentration (at a constant HLR) affect the relative contribution of the microbial reactions to organic matter removal. CWM1 describes the most relevant aerobic, anoxic and anaerobic bio-kinetic processes occurring in HF and VF CWs. CWM1 consists of 17 processes and 16 components in subsurface flow CWs and it is expected CWM1 will become a widely accepted model

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formulation for biochemical transformation and degradation processes in subsurface flow CWs (Langergraber et al. 2009). A brief comparison of the existing numerical modeling software's in CWs is shown in Table 1.

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## 4. Summary and conclusions

It is generally accepted that the CWs may enable the effective, economical and ecological treatment of agricultural, industrial and municipal wastewater. The first-order model is still widely recognized for the design of CWs (Kadlec and Wallace, 2009). Monod kinetics is probably better to describe the biological processes in wetlands (Mitchell and McNevin, 2001). Time dependent retardation model, i.e. TIS model has its unique features. However, none of these models explains the internal process mechanisms and therefore all these models fall under the category of "black-box" models. Statistical technique can be adopted while analyzing the data obtained from CWs. ANN and SOM all show huge promise and are recommended for further scientific studies. The fundamental scientific knowledge of pollutant processes, which takes place within the system, is highly limited. Technical and scientific processes studied are geared towards the media and pollutant interactions in the CW system. FITOVERT, CW2D, STELLA, PHWAT, 2D mechanistic model, CWM1 modeling software's/simulation tool can be used to explain the mathematical processes equations in a better way. From the current review, it is evident that the future direction of CW modeling work should be focused to quantify the rates of individual processes which are happening inside the system. The individual reaction rate constants and the percentage of removal by various mechanisms are vital because it provides valid information to the designers for the efficient design of CWs. Once such kind of information is available, design recommendation can be made for sizing and the pollutant removal can be estimated in great detail. However, process based models for the removal of pollutants in the CWs is still in its infant stage and more technical and scientific study is required to improve the understanding of these complex processes. Considering the fact that time constants of certain microbial and physical chemical reactions range between seconds and hours, calibration probably requires large, high frequency data sets. On the other hand, emphasis should be given to hydraulics of mechanistic model for reliable simulation of CWs. In addition the relationship between dispersivity and saturation degree should also be included in the process-based model because of the variation in water content dynamically during the standard operation (Giraldi et al. 2010). Therefore, it is highly recommended to develop a process based model which can explain the various processes occurring within the wetland system.

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692	List of Figures	
693	Fig. 1 Schematic illustration of wetlands process	
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## **Table captions**

# Table 1 Brief comparison of the existing modeling software's in CWs

Name	Source	Comments
FITOVERT- Version 0.1	University of Pisa, Italy	Newly developed software for VSSF-CW
HYDRUS (CW2D)	PC progress http://www.pc-progress.com	Developed as an extension of HYDRUS 2D
STELLA	High performance systems http://www.hps-inc.com	Lots of users, most used in academic and business and research
PHWAT	Ecole Polytechnique Federale De Lausanne (EPFL),Switzerland	A new module for an existing coupled flow and reactive transport code- PHWAT was implemented
2D Mechanistic Model	Technical University of Catalonia, Spain	2D simulation model is based on the code RetrasoCodeBright (RCB)
CWM1	University of Natural Resources and Applied Life Sciences, Vienna	Mainly used by researchers working in CWs

# **Figure**

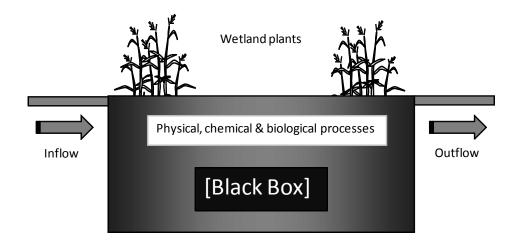


Fig. 1 Schematic illustration of wetlands process