



## Research article

# Modelling bioclogging in variably saturated porous media and the interactions between surface/subsurface flows: Application to Constructed Wetlands



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## ABSTRACT

Horizontal subsurface Flow Constructed Wetlands (HF CWs) are biofilters planted with aquatic macrophytes within which wastewater is treated mostly through contact with bacterial biofilms. The high concentrations of organic carbon and nutrients being transported leads to high bacterial biomass production, which decreases the flow capacity of the porous material (bioclogging). In severe bioclogging scenarios, overland flow may take place, reducing overall treatment performance. In this work we developed a mathematical model using COMSOL Multiphysics™ and MATLAB® to simulate bioclogging effects in HF CWs. Variably saturated subsurface flow and overland flow were described using the Richards equation. To simplify the inherent complexity of the processes involved in bioclogging development, only one bacterial group was considered, and its growth was described using a Monod equation. Bioclogging effects on the hydrodynamics were taken into account by using a conceptual model that affects the value of Mualem's unsaturated relative permeability. Simulation results with and without bioclogging were compared to showcase the impact of this process on the overall functioning of CWs. The two scenarios rendered visually different bacteria distributions, flow and transport patterns, showing the necessity of including bioclogging effects on CWs models. This work represents one of the few studies available on bioclogging in variably saturated conditions, and the presented model allows simulating the interaction between overland and subsurface flow occurring in most HF CWs. Hence, this work gets us a step closer to being able to describe CWs functioning in an integrated way using mathematical models.

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## 1. Introduction

Constructed Wetlands (CWs) are a group of wastewater treatment technologies designed to mimic and intensify pollutants' removal potential of natural wetlands. Like most subsurface environments, the granular material of these systems is prone to clogging (Knowles et al., 2011). This phenomena is responsible for severe changes in the hydrodynamic properties of the granular media i.e. the reduction of both porosity and hydraulic conductivity which result in the proliferation of overland flow (Knowles et al., 2010; Nivala et al., 2012; Pedescoll et al., 2009; Soleimani et al., 2009). Mechanisms responsible for clogging in CWs include

biofilm growth, chemical precipitation, filtration and plant roots development (Knowles et al., 2011; Suliman et al., 2006). After several years of clogging development, this phenomena can cause the complete failure of CWs. Accordingly, clogging is generally referred to as the main operational problem of CWs (Knowles et al., 2011; Pedescoll et al., 2011).

The experimental study of clogging is complex due to the number of parameters involved, their non-linear cross-influence, the ability to observe non-destructively, and the slow rate of the involved processes (it may take many years for a filter to be completely clogged). Consequently, mathematical models are of great help to study clogging, as they allow observing the outcome of complex systems in various experimental conditions (Oberkampf and Trucano, 2002) and enable a better understanding of the involved processes.

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### List of symbols

$C_k$	Concentration of dissolved species $k$ , $\text{mg L}^{-1}$	$th$	Biofilm thickness, $\text{m}$
$D$	Hydrodynamic dispersion tensor, $\text{m}^2 \text{d}^{-1}$	$U$	Mostafa and van Geel (2007)'s flow reduction factor, –
$D_{WB}$	Depth of the Wetland Body subdomain, $\text{m}$	$u$	Specific discharge, $\text{m d}^{-1}$
$h$	Hydraulic head, $\text{m}$	$V_m$	Biomass volume per cubic meter, $\text{m}^3 \text{m}^{-3}$
$K$	Hydraulic conductivity, $\text{m d}^{-1}$	$W_{WB}$	Width of the Wetland Body subdomain, $\text{m}$
$k_r$	Relative hydraulic conductivity, –	$X$	Concentration of bacteria biomass, $\text{mg L}^{-1}$
$K_{sat}$	Saturated hydraulic conductivity, $\text{m d}^{-1}$	$x_{CM}$	x coordinate of the center of mass of bacteria, $\text{m}$
$k_X$	Decay rate of $X$ , $\text{d}^{-1}$	$y_{CM}$	y coordinate of the center of mass of bacteria, $\text{m}$
$K_{X,C}$	Saturation/inhibition coefficient of $X$ by $C$ , $\text{mg L}^{-1}$	$Y_{X,C}$	Yield coefficient for bacteria $X$ on substrate $C$ , $\text{d}^{-1}$
$L_{WB}$	Length of the Wetland Body subdomain, $\text{m}$	$\alpha$	van Genuchten parameter, $\text{m}^{-1}$
$m$	van Genuchten parameter ( $m = 1 - (1/n)$ ), –	$\alpha_T$	Transverse dispersivity, $\text{m}^2 \text{s}^{-1}$
$N_i$	Number of pores of radius $r_i$ , –	$\alpha_L$	Longitudinal dispersivity, $\text{m}^2 \text{s}^{-1}$
$n$	van Genuchten parameter, –	$\beta$	Water contact angle within the tube walls, –
$P_c$	Soil capillary pressure, $\text{Pa}$	$\mu_X$	Maximum specific growth rate of $X$ , $\text{d}^{-1}$
$r_{C_k}$	Reaction rate of $C_k$ , $\text{mg L}^{-1} \text{d}^{-1}$	$\rho_X$	Density of bacteria $X$ , $\text{kg m}^{-3}$
$r_i$	Radius of capillaries filled with water at $P_c$ , $\text{m}$	$\sigma$	Water surface tension, $\text{N m}^{-1}$
$s_{C_k}$	Sources or sinks of $C_k$ , $\text{mg L}^{-1} \text{d}^{-1}$	$\sigma(h)$	Specific volumetric storability, $\text{m}^{-1}$
$S_e$	Specific water saturation, –	$\theta$	Liquid volume fraction, $\text{m}^3 \text{m}^{-3}$
$t$	Time, $\text{d}$	$\theta_r$	Residual liquid volume fraction, $\text{m}^3 \text{m}^{-3}$
		$\theta_s$	Saturated liquid volume fraction, $\text{m}^3 \text{m}^{-3}$

To date, modelling of biological clogging (bioclogging) has been the target of many studies in different disciplines, e.g. soil remediation (Seki et al., 2006), groundwater recharge (Greskowiak et al., 2005) and aquifer thermal energy storage (Bonte et al., 2013). Bioclogging modelling requires coupling flow and transport processes to biofilm growth and the subsequent modification of the hydraulic properties.

Historically, biofilm growth has been modelled using three different approaches based on the scale: microcolony models, biofilm models and macroscopic models (Baveye and Valocchi, 1989). Similarly, the changes of the hydraulic properties can be modelled using pore network models, conceptual models, and empirical laws derived from column experiments (Thullner, 2010). Linking results obtained at these different scales remains challenging because, unlike some abiotic parameters, there do not exist upscaling methods for microbial processes (Thullner, 2010). Furthermore, most attempts to simulate bioclogging have been made in saturated conditions, while only a few have focused on variably saturated conditions (Mostafa and van Geel, 2007).

In the field of CWs, only a few attempts have been made to simulate bioclogging (Hua et al., 2013; Knowles et al., 2011; Rousseau et al., 2005) using complex biokinetic models. Brovelli et al. (2009) compared the performances of three bioclogging models derived from the three different approaches mentioned above to experimental data under saturated conditions and concluded that their models were unable to reproduce long-term clogging evolution. Giraldo et al. (2009, 2010) developed a model (FITOVERT) for vertical flow (VF) CWs including a bioclogging model. The latter uses a semiempirical law (Kozeny–Carman's equation) to modify the saturated hydraulic conductivity according to the biomass concentration but does not modify the unsaturated flow properties. Rajabzadeh et al. (2015) built a model in COMSOL Multiphysics™ to reproduce the reduction of the hydraulic conductivity caused by bacterial growth observed from a previous experimental study on a vertical-flow wetland mesocosm (Weber and Legge, 2011). They used a simplified biokinetic model, based on Monod's formulation, that considered a single bacteria group and a single substrate. They used the Brinkman equation to

describe saturated flow through the porous media and the Kozeny–Carman's equation to translate bacterial growth into porosity reduction.

Despite these attempts, there is still little experience on this field and none of them have been able to predict clogging development in long-term scenarios (Nivala et al., 2012). Furthermore, in CWs both saturated and unsaturated sites exist, and when severe clogging occurs, surface flow also develops. Therefore, to simulate bioclogging and its effects on the hydraulic and hydrodynamic functioning of CWs using numerical models, flow under these three conditions must be considered.

In this work we aim to present a standalone model to simulate variably saturated subsurface flow, bioclogging produced by a single bacterial group and the subsequent surface flow. Instead of using empirical models (e.g. Kozeny–Carman's equation) to translate bacteria development into porosity and hydraulic conductivity reduction, we used one of the three conceptual models proposed by Mostafa and van Geel (2007). These three conceptual models are among the very few bioclogging models applicable under variably saturated conditions. The one used in this work (Model no. 3) is of microscopic nature (it calculates the biofilm thickness) and uses a flow reduction factor to affect the macroscopic relative permeability obtained with Mualem's equation (Mualem, 1976), following bacterial growth.

Moreover we present and compare simulation results obtained from two numerical experiments: one accounting for the changes on the hydrodynamic properties of the granular media (by including the conceptual bioclogging model) and the other one neglecting them.

This is the first work to present simulation results with a model able to describe bacterial growth, bioclogging in variably saturated conditions and the interactions between overland and subsurface flow in horizontal subsurface flow Constructed Wetlands (HF CWs). The presented model brings us a step closer to being able to simulate the overall functioning of CWs, which will occur once it is combined with a complex biokinetic model. With very few modifications, this model can also be applied to related fields of research.

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