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Effect of bacteria density and accumulated inert solids on the effluent pollutant concentrations predicted by the constructed wetlands model BIO_PORE

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ABSTRACT

Constructed wetlands are a widely adopted technology for the treatment of wastewater in small communities. The understanding of their internal functioning has increased at an unprecedented pace over recent years, in part thanks to the use of mathematical models. BIO_PORE model is one of the most recent models developed for constructed wetlands. This model was built in the COMSOL Multiphysics™ software and implements the biokinetic expressions of Constructed Wetlands Model 1 (CWM1) to describe the fate and transport of organic matter, nitrogen and sulphur in horizontal subsurface-flow constructed wetlands. In previous studies, CWM1 was extended with the inclusion of two empirical parameters (M_{bio_max} and M_{cap}) that proved to be essential to provide realistic bacteria growth rates and dynamics. The aim of the current work was to determine the effect of these two parameters on the effluent pollutant concentrations predicted by the model. To that end, nine simulations, each with a different M_{bio_max}-M_{cap} pair, were launched on a high-end multi-processor computer and the effluent COD and ammonia nitrogen concentrations obtained on each simulation were qualitatively compared among them. Prior to this study, a finite element mesh optimization procedure was carried out to reduce computational cost. Results of the mesh optimization procedure indicated that among the 5 tested meshes of different element size, the mesh utilized for this model in previous studies represented a fair compromise between output accuracy and computation time. Results of the sensitivity analysis showed that the value of M_{cap} has a dramatic effect on the simulated effluent concentrations of COD and ammonia nitrogen, which clearly decreased for increasing values of this parameter. On the other hand, the model output was also sensitive to the values of M_{bio_max}, but its effects were less important and no clear relation could be established between its value and the simulated effluent concentration of COD and ammonia nitrogen.

1. Introduction

Constructed wetlands (CWs) are wastewater treatment systems usually applied for communities of less than 2000PE. This technology provides comparable treatment efficiencies with significantly lower energy and maintenance requirements than conventional technologies (García et al., 2010; Puigagut et al., 2007).

However, and due to the diversity and complexity of the physic-chemical and biological processes occurring within CWs, their functioning is far less well understood than that of activated sludge systems. To bridge this knowledge gap, several mathematical models have been developed in recent years to simulate CWs functioning (Meyer et al., 2014; Samsó et al., 2014).

The BIO_PORE model is one of such models and was developed in COMSOL Multiphysics, a commercial finite elements (FE) simulation platform (Meyer et al., 2014; Samsó et al., 2014; Samsó and García, 2013a,b, 2014). This model aims at describing the hydraulics and hydrodynamics of CWs, as well as the removal of the most common pollutants found in wastewater. To that end, it implements the biokinetic model Constructed Wetlands Model 1 (CWM1) (Langergraber et al., 2009), which describes the fate of organic matter, nitrogen and sulphur. This biokinetic model is based on the formulation of the well-known Activated Sludge Model series (ASMs) for aerobic and anoxic processes (Henze et al.,

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2000) and on the Anaerobic Digestion Model 1 (ADM1) to describe anaerobic processes (Batstone et al., 2002).

In BIO_PORE two logistic functions are added to the original formulation of CWM1, which involve two new empirical parameters: M_{bio_max} and M_{cap} (Samsó and García, 2013a). These two parameters represent, respectively, the maximum microbial biomass (carrying capacity) and the maximum amount of particulate solids that can be maintained in a representative volume of granular material. The function involving M_{bio_max} has already been used in several bioclogging studies (Brovelli et al., 2009) and adds a negative feedback term to the growth of all bacteria groups to prevent their unlimited growth in areas where substrates concentrations are high. On the other hand, the expression involving parameter M_{cap} also adds a negative feedback term to the growth equations, but in this case it decreases the growth rate of bacteria due to the progressive accumulation of inert solids in the pore space of the granular media (Samsó and García, 2014). Our previous studies proved the importance of these two functions in order to obtain realistic bacteria concentrations within the granular media (Samsó and García, 2013a, 2014). As bacterial communities play a major role on the treatment of wastewater in CWs, these two functions also improved the model predictions regarding effluent pollutant concentrations.

However, in these previous studies, although a discussion was made around the impact of parameters M_{bio_max} and M_{cap} on the concentration of solids and the different bacterial groups within the bed, their impact on the effluent pollutant concentrations was not evaluated.

In this study we carried out a sensitivity analysis to identify the individual contributions of the two uncertain input model parameters (i.e., M_{bio_max} and M_{cap}) to the output uncertainty (i.e., effluent pollutant concentrations of COD and ammonia and ammonium nitrogen)(Sin et al., 2009).

Sensitivity analysis methods are generally classified between qualitative and quantitative methods and between local and global techniques, and the choice of the method is generally driven by computational cost (Cariboni et al., 2007).

Most of the sensitivity analysis studies carried out in the field of wastewater treatment modelling are of local nature and use a differential analysis of outputs with respect to parameters (Sin et al., 2011). Local methods, are the simplest ones to sensitivity analysis, and consist on repeatedly varying one parameter at a time (OAT) while holding the others fixed (Hamby, 1994).

These sort of methods, which are employed in the current work, are economical from a computational point of view, but they provide qualitative sensitivity measures (they rank the input factors in order of importance, but do not quantify how much a given factor is more important than another) (Dimov and Georgieva, 2010).

To perform the sensitivity analysis, the BIO_PORE model was used with the same domain, parameter values and initial and boundary conditions than in our previous paper in which the model was calibrated (Samsó and García, 2013a). Due to the large computational cost associated with solving the model for a simulated period of an entire year of operation of a wetland (up to 16 h for dense FE meshes with a current desktop computer), and due to the large number of simulations needed for the current and for further studies, a previous mesh optimization procedure was carried out. The objective of this part of the study was to find the FE mesh which would provide the best compromise between numerical solutions accuracy (lower discretization error) and computational cost.

The two empirical parameters discussed in this work are essential to obtain realistic bacteria concentrations when simulating CWs and this study shows how they affect the effluent pollutant concentrations predicted by the BIO_PORE model. In this work we also exploited the batch and parallel computation functionalities of COMSOL Multiphysics™ on a high-end multi-processor computer which is easily justified by the large number of simulations performed.

Table 1
Description of the components considered in BIO_PORE model. S_i are dissolved species (all in the aqueous phase by definition) and X_i are particulate species (either in aqueous or solid phase).

Componenet	Description	Unit	Phase
S_O	Dissolved oxygen	mg COD $\cdot L^{-1}$	Aqueous
S_F	Soluble fermentable COD	mg COD $\cdot L^{-1}$	Aqueous
S_A	Fermentation products as acetate as COD	mg COD $\cdot L^{-1}$	Aqueous
S_I	Inert soluble COD	mg COD $\cdot L^{-1}$	Aqueous
X_{Sm}	Aqueous slowly biodegradable particulate COD	mg COD $\cdot L^{-1}$	Aqueous
X_{Sf}	Solid slowly biodegradable particulate COD	mg COD $\cdot L^{-1}$	Solid
X_{Im}	Aqueous inert particulate COD	mg COD $\cdot L^{-1}$	Aqueous
X_{If}	Solid inert particulate COD	mg COD $\cdot L^{-1}$	Solid
S_{NO}	Nitrite and nitrate nitrogen	mg N $\cdot L^{-1}$	Aqueous
S_{NH}	Ammonium and ammonia nitrogen	mg N $\cdot L^{-1}$	Aqueous
S_{SO4}	Sulphate sulphur	mg S $\cdot L^{-1}$	Aqueous
S_{H2S}	Dihydrogensulphide sulphur	mg S $\cdot L^{-1}$	Aqueous

2. Methods

The local parameter sensitivity analysis and the mesh optimization procedure were performed using the exact same domain, parameter values and boundary and initial conditions as in Samsó and García (2013a). For this reason, only the basic equations of the BIO_PORE model are described in this section. For an in-depth description of all model equations the reader is referred to the original source. All simulations performed in this study were run for the entire first year of operation of a pilot wetland.

2.1. BIO _PORE model description

2.1.1. Governing equations

In BIO_PORE model, the saturated porous media flow is described using the Darcy equation (Eq. (1)).

$$q_i = -K_{ij}\frac{\partial H}{\partial x_j} \tag{1}$$

where, q_i is the specific discharge $[LT^{-1}]$, K_{ij} is the saturated hydraulic conductivity tensor $[LT^{-1}]$, and $(\partial H/\partial x_j)$ the hydraulic gradient vector (unitless). Since in CWs both saturated and unsaturated conditions coexist, the *Deformed Geometry* node of COMSOL Multiphysics™ was used to dynamically adjust the top boundary of the model domain to the simulated shape and location of the water table.

The fate and transport of the aqueous phase (mobile) wastewater components of CWM1 (Table 1) are described with reactive transport equations, one for each component, in which the reactive term accounts for the production/consumption of the substrate through microbial activity (Eq. (2))(Clement et al., 1998).

$$\frac{\partial C_k}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C_k}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(q_i C_k) + r_r - r_{att} + r_{\det} + s_s \tag{2}$$

where $k = 1, 2 \ldots m$ and m is the total number of aqueous phase species (dissolved and particulate, see Table 1). C_k $[ML^{-3}]$ is the concentration of the kth aqueous phase species, D_{ij} $[L^2T^{-1}]$ is the