Environmental Modelling & Software 102 (2018) 115–119

Contents lists available at ScienceDirect

Environmental Modelling & Software

journal homepage: www.elsevier.com/locate/envsoft

Which are the most sensitive parameters for suspended solids modelling in free water surface constructed wetlands?

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ARTICLE INFO

Article history:
Received 14 March 2017
Received in revised form
7 January 2018
Accepted 16 January 2018

Keywords:
Sensitivity analysis
Mathematical modelling
Suspended solids
Morris method
Eutrophic water

ABSTRACT

A large number of input factors are involved in mechanistic models for constructed wetlands simulation. Proper calibration procedure requires identifying which are the most influential ones in the simulation of main interest outputs. Total suspended solids concentration is an essential component in the simulation of eutrophic water treatment. In this paper, a global sensitivity analysis using the Morris method and scaled elementary effects was performed in order to identify which are the most influential input factors in total suspended solids simulation in free water surface constructed wetlands treating eutrophic water. Results indicated that the most influential one was the sedimentation velocity of total suspended solids, followed by parameters related to the resuspension process caused by wind, which presented non-linear or interaction effects.

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1. Introduction

Constructed wetlands (CWs) are complex systems for treating wastewater where several physical, chemical and biological processes take place. Understanding these processes is needed to optimize the performance of CWs but it is hindered by the large number of processes and their interdependency. In this context, mathematical modelling has been considered a promising tool to increase the understanding of the processes involved in CWs (Samsó et al., 2014).

Several mechanistic models have proven to be helpful for increasing the knowledge about the performance of CWs and optimizing both their design and management. BIO-PORE (Samsó and Garcia, 2013) and HYDRUS Wetland Module (Langergraber and Simunek, 2012) are mechanistic wetlands models formed by a number of sub-models that represents the different elements in a CW and their interactions. Among others, these are the biokinetic model, water flow model, transport model or the wetland plants model.

Biokinetic models describe transformation and degradation processes and are frequently highly parameterized models. The model Constructed Wetland Model Number 1 (CWM1) (Langergraber et al., 2009) contains 59 parameters and the biokinetic model Constructed Wetlands 2D (CW2D) (Langergraber, 2001) is formed by 46 parameters. Therefore, identifying which are the most influential input factors in the simulation of each output is required for achieving properly calibration procedures.

However, mathematical simulations are subject to uncertainty since models are an abstract approximation of reality based on a number of assumptions and sensitivity analysis are useful tools to quantify how any modification in model's input factors affect the model's output (Robles et al., 2014). Furthermore, sensitivity analysis facilitates identifying the most influential input factors of a model and simplifies the calibration procedure. On the other hand, appropriate and rigorous sensitivity analysis allows to reduce practical and theoretical identifiability problems in mathematical models (Durán, 2013). Generally, Type I errors are those that identify non-important parameters as significant, whereas Type II errors recognise important parameters as insignificant.

Total suspended solids (TSS) is a fundamental component in eutrophic water since it presents a strong correlation with turbidity, which is an essential factor in determining the ecological status of the water body (Scheffer et al., 1993). In fact, Scheffer et al. determined that switching from a eutrophic to a good ecological status, or vice versa, is highly dependent on water turbidity.

On this basis, Gargallo et al. (2016) developed a biokinetic model

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https://doi.org/10.1016/j.envsoft.2018.01.015
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for free water surface (FWS) constructed wetlands including TSS as an output. This study included a local sensitivity analysis using the absolute-relative sensitivity function of AQUASIM (Reichert, 1994, 1998). This method calculates changes in simulated components when 100% of the value of one input factor is changed while the values of all other input factors remain invariables in their calibrated values. However, local sensitivity analysis does not determine the effect on model output of simultaneously changing the value of different input factors. Global sensitivity analysis like Morris method of Elementary Effects (EEs) (Morris, 1991) offers this possibility and allows to calculate the fractional contribution of each uncertain input factor to the variance of a model output (Haaker and Verheijen, 2004).

In this study, a global sensitivity analysis based on the Morris method was implemented to a mechanistic model for total suspended solids simulation in free water surface constructed wetlands by means of the biokinetic model developed by Gargallo et al. (2016). This study contributes to focus calibration efforts on most influential input factors.

2. Methods

2.1. Model description

The biokinetic model for FWS wetlands used in this study (Gargallo et al., 2016) simulates TSS concentration as an output (X_{TSS}, mg L^{-1}) by means of 7 processes, i.e. growth, decay, respiration and sedimentation of phytoplankton, sedimentation of TSS and sediment resuspension produced by wind and by avifauna. Table 1 shows stoichiometric matrix and processes rates. Furthermore, resuspension produced by wind was not simulated as a dynamic process, so addition of TSS from sediment to water column by wind (TSS_{res}) was calculated using Eq. (1).

$$TSS_{res}\left(\text{mg l}^{-1}\right) = \alpha \cdot W^{\beta}\,\delta(W, W_o)\left(1 - VC \cdot K_{vegresus}\right) \quad (1)$$

where W (m s^{-1}) is maximum daily wind speed, α (mg s l^{-1} d^{-1} m^{-1}) and β are parameters to be calibrated, $\delta(W,W_0)$ is a step function that determines the periods when the wind-induced waves cause resuspension ($\delta = 0$ if $W < W_o$ and $\delta = 1$ if $W > W_o$), VC is vegetation cover, $K_{vegresus}$ is coefficient for trapping by emergent VC in resuspension processes, X_p (mg Chla·L^{-1}) is phytoplankton biomass, G_{max} (d^{-1}) is maximum growth rate for X_P at 20 °C, θ_G is temperature coefficient for X_P growth, T (°C) is temperature, P_{int} (mg P mg $Chla^{-1}$) is phosphorus accumulated inside the phytoplankton cells, P_{min} (mg P mg $Chla^{-1}$) is minimum P_{int} rate for X_P, P_{max} (mg P mg $Chla^{-1}$) is maximum P_{int} rate for X_P, G_L is light limitation in phytoplankton growth kinetics, K_r (d^{-1}) is X_P decay rate at 20 °C, θ_r is temperature coefficient for X_P decay, K_{resp} (d^{-1}) is X_P respiration rate at 20 °C, θ_{resp} is temperature coefficient for X_P respiration, DO (mg O_2 L^{-1}) is dissolved oxygen concentration, $K_{DO\,Xp}$ (mg O_2 L^{-1}) is saturation coefficient for DO in X_P respiration, v_{sXP} (m d^{-1}) is sedimentation velocity of X_p, H (m) is water depth, v_{sTSS} (m d^{-1}) is sedimentation velocity of TSS, K_{vegsed} is coefficient for trapping by emergent VC in sedimentation processes, K_{avi} (mg m^2 L^{-1} d^{-1}) is coefficient of resuspension by avifauna, N_i is the number of birds in the group *i*, RF_i is resuspension factor of the group of birds *i* and A (m^2) is area of the FWS wetland.

The biokinetic model of Gargallo et al. (2016) was properly calibrated and validated using experimental data from two full-scale FWS wetlands treating eutrophic water from Albufera Lake (València, Spain) for three years. That study revealed that TSS were mainly removed by TSS sedimentation, while resuspension produced by both avifauna and wind introduced a significant amount of suspended material to the water column. However, processes related to phytoplankton (i.e. growth, death, respiration and sedimentation) presented little importance in TSS performance within the studied FWS wetlands.

2.2. Morris method

Morris method entails a properly screening strategy for identifying the most influential input factors in a highly parameterized model (Campolongo et al., 2011) by calculating the Elementary Effects (EE_i) of input factors on the output of a model. This method is based on a randomized one-factor-at-a-time (OAT) design where input factors are varied individually by the same relative amount around the nominal point.

The output variable $y = y(x)$ of a model is defined by the scalar *k*-dimensional function, where *k* is the total number of parameters and input values. This function is defined by a vector $x = \{x_1, x_2 \ldots x_k\}$ with *k* components, x_i, that can take *p* levels in the set {0, 1/(p-1), 2/(p-1) … (p-2)/(p-1),1} that identifies an exact point in the experimental *k*-dimensional domain Ω. This assumes that a range of any *k*-dimensional factors has been scaled to the set levels {0, 1/(p-1), 2/(p-1) … (p-2)/(p-1),1} and the region of experimentation Ω is thus a *k*-dimensional *p*-level grid.

EE_i of the *i*th input factor at given value of x randomly selected in Ω was defined by Morris (1991) as shown in Eq. (2). In order to avoid committing a type I error, Sin and Gernaey (2009) proposed to calculate scaled elementary effects ($SEE_{i,j}$, Eq. (3)) for obtaining a non-dimensional and normalized measurement of EE_i. $SEE_{i,j}$ are especially useful to study models where parameters value differs one or more orders of magnitude.

$$EE_i(y) = \frac{[y(x_1, x_2, \ldots x_{i-1}, x_i + \Delta, x_{i+1}, \ldots x_k) - y(x)]}{\Delta} \quad (2)$$

Table 1
Stoichiometric matrix and processes rates for modelling TSS in the biokinetic model by Gargallo et al. (2016).

	Component → / Process ↓	X_{TSS}	r
1.	Growth of X_P	i_{TSSXp}	$G_{max}\theta_G^{T-20}\left(\frac{P_{int}-P_{min}}{P_{max}-P_{min}}\right)X_P \cdot G_L$
2.	Decay of X_P	$-\,i_{TSSXp}$	$K_r\theta_r^{T-20}X_P$
3.	Respiration of X_P	$-\,i_{TSSXp}$	$K_{resp}\theta_{resp}^{T-20}\frac{DO}{k_{DO\,Xp}+DO}X_P$
4.	Sedimentation of X_P	$-\,i_{TSSXp}$	$\left(\frac{v_{sXp}}{H}\right)X_P$
5.	Sedimentation of X_{TSS}	−1	$\left(\frac{v_{sTSS}}{H}\right)X_{TSS}(1 + VC \cdot K_{vegsed})$
6.	Resuspension by avifauna	1	$K_{avi}\frac{\sum_{i=a}^{i} N_i \cdot RF_i}{A}(1 - VC \cdot K_{vegresus})$

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