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FLUID MECHANICS

A STOCHASTIC NUMERICAL APPROACH CONSIDERING UNCERTAIN-INPUT PARAMETERS FOR PHOSPHORUS REMOVAL IN CONSTRUCTED WETLANDS

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Abstract: A stochastic numerical approach for the operation problem concerning the removal of contaminants in Horizontal Subsurface Flow Constructed Wetlands (HSF CW) is presented. Emphasis is given to uncertain-but-bounded input-parameters, which are considered as interval parameters with known upper and lower bounds. For the treatment of this uncertainty, the Monte Carlo method is used. The proposed methodology consists of applying the Monte Carlo procedure by solving the deterministic problem for each of the data-samples. Atypical case of a HSF CW unit, concerning Total Phosphorus (TP) removal, is used in a numerical example. The reliability of the proposed stochastic approach is proved by comparing the numerical results with available experimental ones.

Key words: Environmental fluid mechanics; constructed wetlands; Total Phosphorus (TP) removal; Monte Carlo method; uncertain-but-bounded input-parameters.

1 Introduction

The use of Constructed Wetlands (CWs) for the urban wastewater treatment is a growing technology, due to the ecological and economical advantages that they provide [1–3]. These systems have the ability to "disappear" dangerous pollutants, by reducing their concentration, with performances which are (for some main pollutants) bigger than 99%. In order to achieve more effective and economical results by using CWs, it is important to investigate their operation by taking into account simulation methods, such as Monte Carlo [4, 5].

In the present study, the above procedure is analyzed in a numerical stochastic way, considering the operation of a HSF CW. Among the essential municipal pollutants, which are usually degradated in a CW, the TP is chosen. It is a challenging

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choice, as the phenomenon of adsorption requires special attention during the simulations. For the numerical treatment of the above problem, the MODFLOW code is used [6, 7], which requires the solution of a system of Partial Differential Equations (PDEs), concerning the ground water flow and the transport and decay of contaminants.

In this work, a stochastic numerical approach concerning TP removal in HSF CWs is presented. The detailed description of these facilities is given in next paragraph 4 and in [8]. In the same CW tanks, a numerical simulation by using the Visual MODFLOW computer code has already been realized [9]. During this simulation, which was based in available experimental data, the optimal values for distribution coefficient K_d and the first-order removal coefficient λ were determined. The description of these parameters is given in next equations (3) and (7). By using these values, the model was calibrated in order to simulate the operation of the CW tanks, under various design operation parameters (f.e. temperature, porosity, hydraulic conductivity).

Furthermore, the phenomenon of adsorption can be described by more than one adsorption models, which are presented in following equations (6)–(9). Another numerical simulation has been realized by [10], in order to determine which adsorption model between the linear Freundlich or the non-linear Langmuir isotherms simulates better the real operation of the HSF CWs. During the calibration of the model, the optimal values for the parameters K_L and $S_{\max}$ (described in the following equation (9)) have been estimated.

The originality and the aim of the present study is to solve of the problem concerning the uncertainty for the values of the input parameters. For this purpose, the input-parameters are considered as interval parameters with known upper and lower bounds, characterized as uncertain-but-bounded parameters [11]. As these values can be different for any problem, it is common to achieve reliably results by using a mean-value estimate of the various uncertain input parameters.

2 THE DETERMINISTIC PROBLEM

The traditional numerical simulation of CW operation is usually treated as a *deterministic* one, based on the solution of the following system of PDEs (1)–(7). This PDE system describes the advection, dispersion and removal of a solute in the three-dimensional (3-D) space, considering sources/sinks, equilibrated adsorption and first-order irreversible kinetic reactions. The relevant PDEs, written in tensorial notation $(i, j = 1, 2, 3)$, are [12]:

$$\frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial h}{\partial x_j}\right) + q_v = S_y\frac{\partial h}{\partial t}\,, \tag{1}$$

$$v_i = -\frac{K_{ij}}{\theta}\frac{\partial h}{\partial x_j}, \tag{2}$$

$$\theta R_d \frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(q_i C) + q_v C_s - \lambda_1 \theta C - \lambda_2 \rho_b S, \tag{3}$$

$$R_d = 1 + \frac{\rho_b}{\theta}\frac{\partial S}{\partial C}, \tag{4}$$

$$\rho_b = (1-\theta)\rho_r, \tag{5}$$

where: K_{ij} is a component of the hydraulic conductivity tensor; h is the hydraulic head; q_v is the volumetric flow rate per unit volume of aquifer, representing fluid sources (positive) or sinks (negative); S_y is the specific yield of the porous materials; v_i is the seepage or linear pore water velocity, which is related to Darcy velocity q_i through the relationship: $q_i = v_i\theta$; θ is the porosity; R_d is the retardation factor; C is the aqueous solute concentration; D_{ij} is the hydrodynamic dispersion coefficient tensor; C_s is the concentration of the source or sink flux; ρ_b is the dry bulk density of the soil; S is the concentration adsorbed by the solid phase of the porous medium; ρ_r is the density of solid grains of the porous material; λ_1 and λ_2 are the removal coefficients for the dissolved and adsorbed phases respectively (usually it is: $\lambda_1 = \lambda_2 = \lambda$).

Equation (3) is linear when the flow of a non-absorbable pollutant (like Biochemical Oxygen Demand) is analysed. For this case, it is $S = 0$ and $R_d = 1$.

When the flow of an absorbable pollutant is investigated, like in present study, equation (3) can be a linear or a non-linear one, as it is $S \neq 0$ and $R_d > 1$. The following cases concerning TP are usually considered [10, 13]:

(a) The *non-linear Freundlich isotherm*:

$$S = K_F C^{\alpha}. \tag{6}$$

The constant K_F and the exponent α are experimentally estimated according to the type of pollutant and the porous medium. When $\alpha \neq 1$, equation (3) becomes non-linear.

(b) The *linear isotherm of Freundlich*, which is usually chosen for pollutants with initial low concentrations:

$$S = K_d C, \tag{7}$$

$$R_d = 1 + \frac{\rho_b}{\theta}K_d; \tag{8}$$

(c) The *non-linear Langmuir isotherm*:

$$S = S_{\max}\frac{K_L C}{1 + K_L C}, \tag{9}$$

where $S_{\max}$ is the maximum adsorption capacity; and K_L is the Langmuir constant.

3 THE STOCHASTIC PROBLEM

The input parameters concerning the various coefficients of the above system of equations (1)–(9) are rarely known in a safe way. For the estimation of the optimal values for these parameters, the Visual MODFLOW computer code is used.

First, the lower and upper bounds for reliable estimates are determined according to the available literature and experimental data. Then, the Monte Carlo simulation is applied and a set of deterministic values for the input parameters is available. Finally, a statistical analysis is followed in order to choose the optimal values for each input parameter.

4 A NUMERICAL EXAMPLE

A representative numerical example concerning the removal of Total Phosphorus (TP) removal in a typical pilot-scale HSF CW tank is presented. The detailed description of this facility is presented in [8]. The problem concerns a pilot-scale unit, as the dimensions of the investigated tank are 3 m length, 0.75 m width and 0.45 m height (Fig. 1). The CW is filled with cobbles (CO) as porous material and is planted with common reed (*Phragmites australis* reed-R). Therefore, the investigated CW tank is symbolized as CO-R.

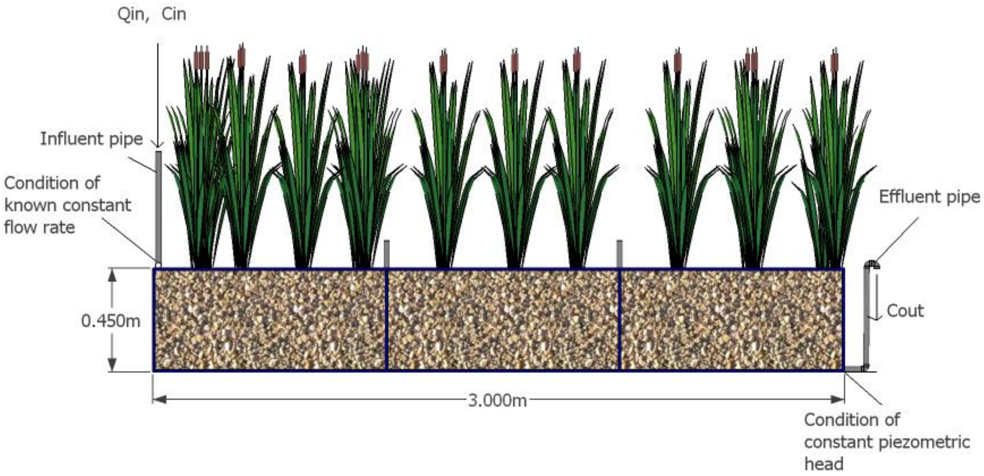

Fig. 1: Schematic section of the investigated HSF CW tank.

As mentioned, available experimental data from the operation of the above pilot-scale HSF CW are used [8]. The mean value of the experimental inlet TP concentration is $C_{\text{in}} = 9.1$ mg/L, while the mean value of the experimental measured outlet TP concentration is $C_{\text{out}} = 5.1$ mg/L. The TP concentration was measured at three places (see Fig. 1) in distances from inlet, i.e., at $x_1 = 1$ m, at $x_2 = 2$ m and at $x_3 = 3$ m (outlet of the tank). The corresponding mean values are 7.3 mg/L, 5.9 mg/L and 5.1 mg/L, respectively. For the simulation, the linear isotherm of Freundlich is used, as this adsorption model has been shown that describes better of the operation of the HSF CWs [10].

The uncertain-but-bounded input parameters for the stochastic analysis are estimated by using available upper (U_B) and lower (L_B) bounds. The bounds for the first-order decay coefficient λ of equation (3) is [8]: $L_B = 0.060$ day^{-1} and $U_B = 0.070$ day^{-1}, i.e., it is:

$$0.05 \leq \lambda \leq 0.07\,. \tag{10}$$

Similarly, the range of appropriate values for the Freundlich distribution coefficient K_d of equation (7) is estimated as follows [10]:

$$0.10 \leq K_d \leq 1.00\,. \tag{11}$$

The hydraulic conductivity K has a LOGNORMAL probability distribution, whereas porosity ε and dispersivity α_L have a NORMAL probability distribution [14]. The first-order decay coefficient λ and the parameter α are considered to have a UNIFORM probability distribution. Thus, for the investigated HSF CW, in Table 1 the truncated Probability Density Functions (PDF) are shown. By COV is denoted the Coefficient of Variation. The mean values are estimated as $(U_B + L_B)/2$.

Table 1: Distribution properties of uncertain-but-bounded input parameters

Input parameters	Distribution (PDF)	Mean value	COV [%]
K [m/sec]	LOGNORMAL	1.742	25
ε [%]	NORMAL	0.555	15
α_L [cm]	NORMAL	2.370	50
λ [day^{-1}]	UNIFORM	0.063	20

In Table 2, the mean values of the obtained stochastic results for the TP concentration ratios C/C_{in} are presented. For the determination of these results, 250 Monte Carlo samples have been used. The above probabilistic results are given in terms of stochastic mean values and COV (Coefficient of Variation) and compared with C/C_{in} corresponding experimental ones [12].

The results of Table 2 show that the relevant numerical stochastic results have a good matching to available experimental ones, as the values of the experimental and the stochastic concentration rations C/C_{in} are similar for each point among CW length.

Table 2: Representative results for the TP concentrations along tank CO-R

Concentration measured points	Experimental mean value C [mg/L]	Experimental mean value C/C_{in} [%]	Stochastic mean value C/C_{in} [%]	COV [%]
$x_1 = 1$ m	7.3	80.22	78.84	11.58
$x_2 = 2$ m	5.9	64.84	65.78	18.84
$x_3 = 3$ m	5.1	56.04	54.87	23.78

5 CONCLUSION

A stochastic approach based on Monte Carlo simulations has been developed for the problem of ground water flow and contaminant removal in constructed wetlands, taking into account uncertain input parameters. In a numerical example concerning TP removal in a typical pilot scale HSF CW tank, the comparison between available experimental results and the computed stochastic ones have shown a very satisfactory agreement. These results are very encouraging for further futural investigations, as the phenomenon of adsorption, which usually creates some problems during the simulation of adsorbed pollutants, did not effect the success of the proposed methodology Thus, the effectiveness and the reliability of the proposed stochastic approach is proven and can be used for CWs tanks, especially with similar operation parameters with the present study.

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