A Computational Investigation of the Optimal Reaction Type Concerning BOD Removal in Horizontal Subsurface Constructed Wetlands

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Keywords: Computational Environmental Engineering; Groundwater Flow; Constructed Wetlands; Biochemical Oxygen Demand; MODFLOW Computer Code; Optimal Reaction Type

1 Introduction

Constructed Wetlands (CW) are recently used in the Environmental Engineering as a good alternative solution for small settlements in order to treat municipal wastewater and to remove groundwater pollutants in contaminated soils [1]. The numerical simulation of CW operation is based on concepts of groundwater flow, contaminant transport and removal through porous media and requires the choice of the optimal reaction type. So it seems necessary to investigate computationally the optimal design characteristics of CW, in order to maximize their removal efficiency and keep their area and construction cost to a minimum.

The present research treats with a numerical simulation of the Biochemical Oxygen Demand (BOD) removal in Horizontal Subsurface Flow Constructed Wetlands (HSF CW). Emphasis is given to select the optimal type of the reaction concerning the BOD removal. For this purpose, a computational investigation is realized by comparing the most usual reaction type, the first-order one [2], and the recently proposed Monod type [3], with simulated experimental data. These data are obtained from five pilot-scale HSF CW units, which were operated for two years in the facilities of the Laboratory of Ecological Engineering and Technology of Democritus University of Thrace, Xanthi, Greece. For more details concerning the description of the pilot-scale units and the experimental procedure, see [2]. For the numerical simulation, the Visual MODFLOW computer code [4] is used, and especially the RT3D code [5] for the Monod type reaction. The comparison between first-order and Monod reaction

types is based on the experimental and computational values of BOD concentration at selected points along the length of the CWs.

2 The mathematical formulation of the problem

The partial differential equation which describes the fate and transport of contaminants of species k without adsorption in 3-D, transient groundwater flow systems can be written, using tensorial notation (i,j = 1,2,3), as follows [6,7]:

$$\frac{\partial(\theta C^k)}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij}\frac{\partial C^k}{\partial x_j}\right) - \frac{\partial}{\partial x_i}\left(\theta v_i C^k\right) + q_v C_s^{\ k} + \sum R_n \qquad (1)$$

where θ is the porosity of the subsurface medium [dimensionless], C^k is the dissolved concentration of species k, in [ML^{-3}], D_{ij} is the hydrodynamic dispersion coefficient tensor, in [L^2T^{-1}], v_i is the seepage or linear pore water velocity, in [LT^{-1}], which is related to the specific discharge or Darcy flux through the relationship: $q_i = v_i\,\theta$, q_V is the volumetric flow rate per unit volume of aquifer representing fluid sources (positive) and sinks (negative), in [T^{-1}], C_s^k *is* the concentration of the source or sink flux for species k, in [ML^{-3}], and ΣR_n is the chemical reaction term, in [$ML^{-3}T^{-1}$].

The above Equation (1) is the governing equation underlying in the transport model and contaminant removal. The required velocity v_i is computed through the Darcy relationship:

$$v_i = -\frac{K_{ij}}{\theta}\frac{\partial h}{\partial x_j} \qquad (2)$$

where K_{ij} is a component of the hydraulic conductivity tensor, in [LT^{-1}], and h is the hydraulic head, in [L].

The hydraulic head $h = h(x_i;t)$ is obtained from the solution of the three-dimensional groundwater flow equation:

$$\frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial h}{\partial x_j}\right) + q_v = S_y\frac{\partial h}{\partial t} \qquad (3)$$

where S_y is the specific yield of the porous materials and q_v is the volumetric flow rate per unit area of aquifer, representing fluid sources (positive) and sinks (negative) when precipitation and evapotranspiration effects are taken in to account, respectively, in [LT^{-1}]

As concerns the reaction term ΣR_n in Equation (1), the optimal type according to available experimental data must be chosen. For the usual linear reaction case, this term depends on the first-order removal coefficient λ and is given by the formula:

$$\Sigma R_n = -\lambda\theta Cn \qquad (4)$$

For non-linear reaction cases, the Monod reaction type has been alternatively proposed recently [3]. Then, the following formula is used for the reaction term:

$$\Sigma R_n = -K_{max}\frac{C}{K_s+C} \qquad (5)$$

where K_{max} is the zero-order removal capacity, in [$ML^{-3}T^{-1}$], and K_s is the half-saturation constant for the considered contaminant, in [ML^{-3}].

So, the above Equations (1)-(3), combined with either, Equation (4) or (5), and appropriate initial and boundary conditions, describe the 3-dimensional flow of groundwater and the transport and removal of contaminants in a heterogeneous and anisotropic medium. Thus, for the case of one only ($k = 1$) pollutant species, the unknowns of the problem are the following five space-time functions: The hydraulic head: $h = h(x_i;t)$, the three velocity components: v_i and the concentration: $C = C(x_i;t)$.

The problem is linear when the reaction Equation (4) for the first-order type is used, whereas becomes a non-linear one when the reaction Equation (5) for the Monod type is used.

3 The numerical treatment of the problem

For the numerical solution of the problem which was described in previous paragraph, the Finite Difference Method is chosen among the other available numerical methods. The reason is that the CW usually have a rectangular scheme. This method is the basis for the computer code family MODFLOW, which is widely used for the simulation of groundwater flow and mass transport, see e.g. [2, 6]. In the present study, the MODFLOW code, accompanied by the effective computer packages MT3DMS and RT3D modules, is used. RT3D is a general purpose, multispecies, reactive transport code. The double Monod model will be applied, where BOD is the electron donor and oxygen is the electron acceptor.

4 Preliminary results and conclusions

The optimal choice of the reaction type concerning BOD removal has been computationally investigated for the tank which is planted with common reed and contains medium gravel as porous medium (MG-R), see [2]. The hydraulic residence time (*HRT*) is 14 days.

The herein proposed numerical approach has been applied and first representative results are shown in the Fig. 1. Comparison curves concerning the concentrations along the tank axis and based on the available experimental results (C_{exp}), the first-order reaction type (C_{first}), the Monod kinetics (C_{Monod}) and the zero-order reaction type are depicted. It is concluded that the optimal reaction type, approaching in the best way the experimental results, is the first-order reaction.

As the results show, the proposed numerical approach can be applied effectively for the optimal choice of the reaction type. This approach will be extended in forthcoming research for the case of multiple interacting contaminants.

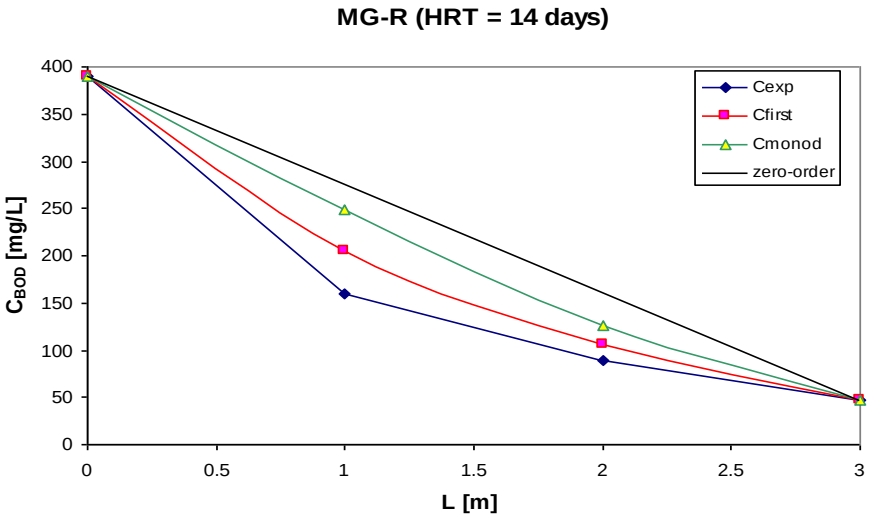

Fig. 1. Comparison curves for the BOD removal in the unit MG-R concerning the experimental results, the first-order reaction type, the Monod kinetics and the zero-order reaction type.

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