

# Mathematical modelling of nitrogen removal in horizontal subsurface flow constructed wetland

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**ABSTRACT.** The research work presented herein makes a contribution to HSSF CW grey-water treatment by developing a conceptual and numerical model to simulate the spatial and temporal variations of nitrogen concentration. This paper presents the simulation of flow and nitrogen removal processes by using the advection-dispersion-reaction modeling approach. The flow equation is solved by using the mixed finite element method. The system of advection-dispersion-reaction is solved by using the technique of separation of the operators. The equation of advection is approximated by the Characteristics-Galerkin Method. The dispersion-reaction equation was carried by using the finite element method. The softwares `freefem++` and `matlab` were used. This phenomenon was materialized by a horizontal subsurface Flow Constructed Wetland treating greywater in a Moroccan primary school. The decay coefficient are been identified by solving an inverse problem using observed data. The Particle Swarm Optimization and Gravitational Search Algorithm (PSOGSA) proposed by Mirjalili et al. [24] is used to solve the inverse problem. Numerical simulation was validated after calibration on the basis of obtained experimental data by controlling water quality parameters over a period of 100 days. Comparative analysis shows that the total predicted effluent of nitrogen concentration obtained by the numerical simulation agrees fully with the one obtained by experimental data.

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## 1. Introduction

The processes that govern the transformation of nitrogen compounds in artificial marshes are multiple and refer to the nitrogen cycle in porous media. For the sake of synthesis, the complex processes related to the fixation of atmospheric nitrogen by plants and free bacteria of the filter substrate will not be developed. Only the phenomena of degradation of the nitrogen compounds contained in the wastewater will be exposed.

Nitrogen supplied to artificial wetlands by wastewater is usually in organic form. It undergoes ammonification, then nitrification and finally denitrification according to the biochemical conditions of the environment ([30], [5], [20]).

Ammonization consists of the mineralization of organic nitrogen into ammonia ( $\text{NH}_3$ ) under the action of a living heterotrophic bacterial flora in the filtration substrate. It occurs in both aerobic and anaerobic environments. In turn, the ammonia undergoes various transformations to give ammonium ( $\text{NH}_4^+$ ).

In recent years, constructed wetland (CW) has become a major way of groundwater treatment. In [23], Mouaouia et al. studied mathematical modeling and numerical simulation of the evolution of phosphorus concentration in a Wetland treating Grey-water Constructed at a primary school of Marrakesh.

The aim of this work is to increase the understanding of the nitrogen removal in the same system.

The model focuses on water flow and reactive solute transport. Nitrogen is present in wastewater as ammonium,  $\text{NO}_2^-$  and  $\text{NO}_3^-$ . The mathematical model that governs the evolution of the concentrations is a system of hierarchical equations of convection-dispersion-reaction. This system of equations is coupled with the hydraulic head equation.

The structure of our paper is outlined as follows. In Section 2 the mathematical modeling is introduced, Existence and uniqueness of the solution of hierarchical equations of convection-dispersion-reaction used is presented. In Section 3 is devoted to the numerical resolution of the equations. The section 4 present the inverse problem. Existence and uniqueness of this problem have been established. In Section 5 we present Particle Swarm Optimization and Gravitational Search Algorithm (PSOGSA) used to solve inverse problem. The results and discussion of numerical experiments are presented in Section 6.

## 2. Mathematical modeling

**2.1. Experimental data.** To meet the objectives of this research, a HSSF CW was built at a Primary school in Marrakesh (Morocco) ( $31^\circ 42' 24'' \text{N}$ ,  $7^\circ 58' 05'' \text{W}$ , 451m), with an average annual temperature of  $19.6^\circ\text{C}$  and annual precipitation of 282 mm. At the upstream of the HSSF, all the school grey water was collected from hand wash sinks and directed to a pre-treatment unit.

In order to evaluate the performance of simulation approaches and mathematical models, experimental data were taken. We took measures at the inlet and the outlet every five days.

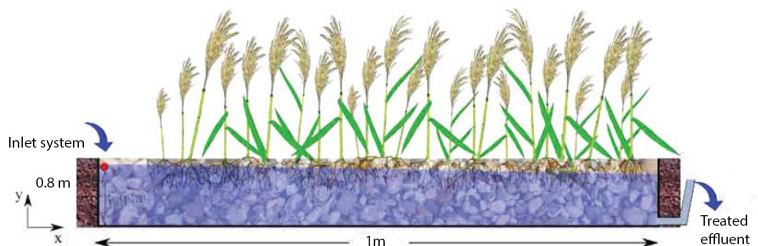


FIGURE 1. Site.

**2.2. Mathematical modeling of flow.** In order to obtain the experimental data for this study, we used a HSF CW similar to those find in the paper of Akratos and Tsihrintzis [1]. Our facility is a rectangular tank (with dimensions 5 m long, 0.75 m wide and 0.6 m deep). Three different porous media layers were used, namely medium gravel (MG), fine gravel (FG) and cobbles (CO). Each one represents a full compartement of 0.2m tickness and 5m long. The tank is planted using the cattails (*C, Typha latifolia*). Regarding other data for the CW layers, we have the following values respectively for MG, FG and CO: porosity( $\omega$ ) 0.39, 0.33 and 0.29, permeability( $K$ ) :  $10^{-7}m^2, 6.25 \cdot 10^{-7}m^2$ , and  $2.25 \cdot 10^{-5}m^2$ .

**2.2.1. Condition of flow.** Wastewater enters the domain through boundary 3 (a length of 0.2 m in the  $x^{th}$  direction representing the mixing zone) where a constant hydraulic head of 0.6 m is defined and the effluent leaves through boundary 5 (a length of 0.1 m in the  $y^{th}$  direction), where a constant hydraulic head of 0.4 m is defined. Boundaries 1, 2, 4 and 6 represent a null flux.

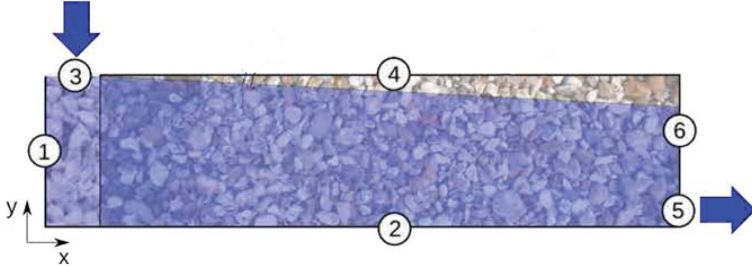


FIGURE 2. Conditions of flow.

**2.2.2. Mathematical model.** Under the above mentioned flow conditions and applying the mass conservation law and the Darcy's law ([18, 21]), the flow in transitory mode in the domain is governed by the following system of equations:

$$\left\{ \begin{array}{ll} S(x, y) \frac{\partial h(x, y, t)}{\partial t} - \text{div}(K(x, y) \cdot \nabla h(x, y, t)) = f(x, y, t) & \text{in } \Omega \times ]0, T[ \\ h(x, y, 0) = h_0(x, y) & \text{in } \Omega \\ h(x, y, t) = h_D(x, y, t) & \text{on } \Gamma^D \times ]0, T[ \\ -K(x, y) \frac{\partial h(x, y, t)}{\partial n} = h_N(x, y, t) & \text{on } \Gamma^N \times ]0, T[ \end{array} \right. \quad (1)$$

where

- $T$  is the date of measure.
- $\Omega$ , representing the domain
- $h$  is the hydraulic potential
- $f$  is the source term
- $h_0$  the initial condition corresponding to the date  $t = 0$
- $h_D$  is the Dirichlet boundary condition, representing the imposed potential
- $\Gamma^N$  represent boundaries 1, 2, 4 and 6
- $\Gamma^D =$  represent boundaries 3 and 5

- $K$  and  $S$  represent respectively the permeability function and the coefficient of storage.

Once the equation (1) is resolved, let  $h$  denote this solution, we deduce respectively the Darcy's velocity  $u$  and the velocity by the following relations:

$$\begin{aligned} u(x, y, t) &= -K(x, y) \cdot \nabla h(x, y, t) & \text{in } \Omega \times [0, T] \\ v(x, y, t) &= \frac{u(x, y, t)}{\omega} & \text{in } \Omega \times [0, T] \end{aligned} \quad (2)$$

where  $\omega$  is the effective porosity.

### 2.3. Transport modeling.

**2.3.1. Mathematical model.** The evolution of the contaminant concentration is governed by the reaction-adsorption-diffusion following equation ([18, 21]):

$$\begin{cases} \frac{\partial C}{\partial t} = \nabla \cdot (D \cdot \nabla C) - \nabla \cdot (vC) - \lambda C & \text{in } \Omega \times ]0, T[ \\ C(x, y, 0) = C_0(x, y) & \text{in } \Omega \\ -D \frac{\partial C}{\partial n} + (v \cdot n)C = 0 & \text{on } \Gamma^0 \times ]0, T[ \end{cases} \quad (3)$$

where:

- $C$  the concentration ( $ML^{-3}$ ),
- $C_0$  the initial concentration ( $ML^{-3}$ ),
- $D$  the dispersion tensor ( $L^2T^{-1}$ ),

$$D = \begin{pmatrix} D_{xx} & D_{xy} \\ D_{yx} & D_{yy} \end{pmatrix}$$

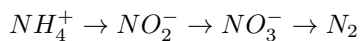
- $\lambda$ , the decay coefficient constant ( $T^{-1}$ )
- $v$  the velocity
- $\Gamma^0$  represent boundaries 1,2,3,4,5 and 6.

A general dispersion tensor  $D$  is given by

$$\begin{aligned} D_{xx} &= \frac{\alpha_L v_x^2 + \alpha_T v_y^2}{\sqrt{v_x^2 + v_y^2}} + D_m, \\ D_{yy} &= \frac{\alpha_L v_y^2 + \alpha_T v_x^2}{\sqrt{v_x^2 + v_y^2}} + D_m, \\ D_{xy} = D_{yx} &= (\alpha_L - \alpha_T) \frac{v_x v_y}{\sqrt{v_x^2 + v_y^2}}, \end{aligned}$$

where  $\alpha_L$  and  $\alpha_T$  is the longitudinal and transverse dispersivities (L),  $D_m$  is the molecular diffusion ( $L^2T^{-1}$ ). The last term to the right is the sink-source term  $R$  used for the simulation of chemical reactions. He takes't account plant uptake, substrate adsorption and desorption. This term usually depends on the concentrations of the reagents involved in the chemical reaction, in this case is expressed by the simple relation:  $R = -\lambda C$ , where  $\lambda$  is a coefficient of decomposition.

Nitrogen is present in wastewater as ammonium,  $NO_2^-$  and  $NO_3^-$  with concentrations respectively denoted as  $c_1, c_2$  and  $c_3$ . We assume that the kinetics of nitrogen simulated by the following reaction chain (nitrification denitrification):



where  $N_2$  represents nitrogen in gaseous form, which is removed from the system. Under these conditions, the concentrations of the substances in the bio-reactor are governed by the following system of equations:

$$\left\{ \begin{array}{ll} l \frac{\partial c_1}{\partial t} = \nabla \cdot (D \cdot \nabla c_1) - \nabla \cdot (v c_1) - \lambda_1 c_1 & \text{in } \Omega \times ]0, T[, \\ \frac{\partial c_2}{\partial t} = \nabla \cdot (D \cdot \nabla c_2) - \nabla \cdot (v c_2) + \lambda_1 c_1 - \lambda_2 c_2 & \text{in } \Omega \times ]0, T[, \\ \frac{\partial c_3}{\partial t} = \nabla \cdot (D \cdot \nabla c_3) - \nabla \cdot (v c_3) + \lambda_2 c_2 - \lambda_3 c_3 & \text{in } \Omega \times ]0, T[, \\ c_i(x, y, 0) = c_i^0(x, y) & \text{in } \Omega, i \in \{1, 2, 3\}, \\ -D \frac{\partial c_i}{\partial n} + (v \cdot n) c_i = 0 & \text{on } \Gamma^0 \times ]0, T[, i \in \{1, 2, 3\}. \end{array} \right. \quad (4)$$

This mathematical model (4) was originally proposed by Cho (1971). In a particular case, van Genuchten (1985) gave an analytical solution. The application of this model to simulate processes in constructed wetlands was first used by Akratos and Tsihrintzis [1], using experimental data. They validated the performance of these approaches by comparing the results of the simulation with existing experimental data from five pilot-scale CW facilities containing different vegetation and porous material types. The characteristic values of the disintegration coefficients  $\lambda_i$  are estimated, which incorporate the influence of vegetation and temperature and are useful in the design of constructed wetlands or the simulation of nitrogen fate in geological formations.

### 3. Numerical modeling

**3.1. Equation of flow solving.** In this part, we propose to solve numerically the equation (1) by using the finite element method for the space discretization. A implicit scheme of Euler will be used for the temporal discretization.

By using a implicit scheme of Euler on the equation (1), we obtain

$$\left\{ \begin{array}{ll} S \frac{h^{n+1} - h^n}{\Delta t} - \text{div}(K \nabla h^{n+1}) = f^{n+1} & \text{in } \Omega \\ h^{n+1} = h_D & \text{on } \Gamma^D, n = 0, \dots, M-1. \\ -K \frac{\partial h^{n+1}}{\partial \nu} = h_N & \text{on } \Gamma^N \end{array} \right. \quad (5)$$

Deduce the Darcy's velocity

$$u^{n+1}(x, y) = -K(x, y) \cdot \nabla h^{n+1}(x, y),$$

where  $\Delta t$  is the step of time giving by  $\Delta t = \frac{T}{M}$ ,  $t_n = n \frac{T}{M}$  and  $f^n = f(x, y, t_n)$ , ( $M$  a integer strictly positive).

Let's suppose:

$$\mathcal{V} = \{ \psi \in H^1(\Omega); \psi = 0 \text{ on } \Gamma^D \}.$$

Since  $\text{mes}(\Gamma^D) > 0$ , according to [8], we can choose

$$\| \psi \|_V = \left( \int_{\Omega} |\nabla \psi|^2 \right)^{1/2} \text{ as norm on } V.$$

Let  $\psi \in \mathcal{V}$  be a test function. Multiplying (5) by  $v$  and integrating by parts, the variational formulation associated to the problem (5) is given by

$$\left\{ \begin{array}{l} \text{find } h^{n+1} \in H^1(\Omega) \text{ with } h^{n+1} = h_D \text{ on } \Gamma^D \text{ such that } \forall \psi \in V \\ \int_{\Omega} \beta h^{n+1} \psi + \int_{\Omega} K \nabla h^{n+1} \cdot \nabla \psi = \int_{\Omega} \beta h^n \psi + \int_{\Omega} \beta f^{n+1} \psi + \int_{\Gamma^N} h_N \psi \end{array} \right. \quad (6)$$

where  $\beta = \frac{S}{\Delta t}$ . Thus the theorem of Lax-Milgram ensures the existence and uniqueness of a solution to the variational problem (6) and consequently the existence and uniqueness of a solution of (5).

We denote by  $\gamma_d$  the trace operator. Let  $r_d \in H^1(\Omega)$  such as  $\gamma_d(r_d) = h_D$  and we denote  $h_d^{n+1} = h^{n+1} - r_d$ .

Let  $T_h$  be a triangulation of  $\Omega$  and we denote  $P_1$  the space of continuous piewise affine function in  $\Omega$  i.e the space of continuous functions which are affine in  $x, y$  on each triangle of  $T_h$ . We pose  $V_h = P_1 \cap V$ .  $V_h$  is a linear vector space of finite dimension. We denote  $N$  its dimension and  $\phi_1, \dots, \phi_N$  a basis. The approximated problem is:

$$\text{find } \tilde{h}^{n+1} \in V_h, \text{ such that } \tilde{h}^{n+1}(x, y) = \sum_{i=1}^N h_i \phi_i(x, y), \quad (7)$$

and take  $\tilde{h}^{n+1} = h^{n+1}$  and  $v = \phi_i$  for  $i = 1, \dots, N$ , we remark that (7) is equivalent to the resolution of the linear system

$$AX = B \quad (8)$$

where  $X = (h_i)_{i=1, \dots, N}$ ,

$$A_{ij} = \int_{\Omega} \beta \phi_i \phi_j + \int_{\Omega} K \nabla \phi_j \cdot \nabla \phi_j = \sum_{T \in T_h} \int_T \beta \phi_i \phi_j + \int_T K \nabla \phi_j \cdot \nabla \phi_j$$

and

$$\begin{aligned} B_i &= \int_{\Omega} \beta h^n \phi_i + \int_{\Omega} \beta f^{n+1} \phi_i + \int_{\Omega} K \nabla r_d \cdot \nabla \phi_i + \int_{\Omega} \beta r_d \phi_i + \int_{\Gamma^N} h_N \phi_i \\ &= \sum_{T \in T_h} \int_T \beta h^n \phi_i + \int_T \beta f^{n+1} \phi_i + \int_T K \nabla r_d \cdot \nabla \phi_i + \int_T \beta r_d \phi_i + \int_{T \cap \Gamma^N} h_N \phi_i. \end{aligned}$$

**3.2. Equation of transport solving.** We used operator splitting, [14, 10]. The transport equation (3) is divided into two distinct equations.

At each step of time, we solve firstly by using Characteristics-Galerkin Method the equation of advection.

$$\begin{cases} \frac{\partial C_{i,a}^k}{\partial t} + \text{div}(v C_{i,a}^k) = 0 & \text{in } \Omega \times ]0, T[, \\ C_{i,a}^k(x, y, 0) = C^{k-1} & \text{in } \Omega. \end{cases} \quad (9)$$

We obtain a solution that we note  $C_{i,a}^k$ .

And secondly, We used implicit finite difference method for the discretization of the time variable and a discretization in finite element  $P_1$  for the space to approximate dispersion-reaction equation

$$\begin{cases} \frac{\partial C_i^n}{\partial t} - \text{div}(D \nabla C_i^n) + \lambda_i C_i^n = f_i & \text{in } \Omega \times ]0, T[, \\ C_i^n(x, y, 0) = C_{i,a}^k & \text{in } \Omega, \\ -D \frac{\partial C_i^n}{\partial n} + (v C_i^n) \cdot n = C_{i,a}^n & \text{on } \Gamma^N \times ]0, T[. \end{cases} \quad (10)$$

The parameters  $\lambda_i$ ,  $i \in \{1, 2, 3\}$  are been identified by solving an inverse problem using data observed.

#### 4. Identification of parameters

In this section, we focus on the identification of parameters, so we formulate our problem to a minimization problem, after we present the derivative in order to make some numerical example. Let's start by the minimisation problem.

**4.1. Minimization problem.** Throughout this section we are interesting in the following minimization problem

$$\min_{\Lambda \in D \subset \mathbb{R}^3} J(\Lambda), \quad (11)$$

the cost functionnal  $J$  is given by a least square criterion

$$J(\Lambda) = \frac{1}{2} \sum_{i=1}^3 \int_0^T \int_{\Omega} (c_i - c_i^{obs})^2 d\sigma dt$$

where  $C = (c_1, c_2, c_3)$  solution of (4),  $c_i^{obs}$  is the data observed and  $\Lambda = (\lambda_1, \lambda_2, \lambda_3)$  the vector of parameters.

**Theorem 4.1.** *Suppose that  $0 < a \leq \lambda_i \leq b$ ,  $i \in \{1, 2, 3\}$ . The function  $J$  defined by*

$$\begin{aligned} J : [a, b]^3 &\longrightarrow \mathbb{R} \\ \Lambda = (\lambda_1, \lambda_2, \lambda_3) &\longmapsto \frac{1}{2} \sum_{i=1}^3 \int_0^T \int_{\Omega} (c_i - c_i^{obs})^2 dx dt \end{aligned}$$

is differentiable with respect to  $\Lambda$  and for all  $\xi = (\xi_1, \xi_2, \xi_3) \in [a, b]^3$ , we have

$$\nabla J(\Lambda) \cdot \xi = \int_{T_{j-1}}^{T_j} \int_{\Omega} \left( \xi_1 c_1 (p_1 - p_2) + \xi_2 c_2 (p_2 - p_3) + \xi_3 c_3 p_3 \right)$$

with  $(c_1, c_2, c_3)$  is solution of (4) and  $(p_1, p_2, p_3)$  is solution of the following problem

$$\left\{ \begin{array}{ll} -\frac{\partial p_1}{\partial t} = \nabla \cdot (D \cdot \nabla p_1) - \nabla p_1 \nabla v + \lambda_1 p_2 - \lambda_1 p_1 + c_1^{obs} - c_1 & \text{in } \Omega \times ]0, T[, \\ -\frac{\partial p_2}{\partial t} = \nabla \cdot (D \cdot \nabla p_2) - \nabla p_2 \nabla v + \lambda_2 p_3 - \lambda_2 p_2 + c_2^{obs} - c_2 & \text{in } \Omega \times ]0, T[, \\ -\frac{\partial p_3}{\partial t} = \nabla \cdot (D \cdot \nabla p_3) - \nabla p_3 \nabla v - \lambda_3 p_3 + c_3^{obs} - c_3 & \text{in } \Omega \times ]0, T[, \\ p_i(x, y, T) = 0 & \text{in } \Omega, i \in \{1, 2, 3\}, \\ D \frac{\partial p_i}{\partial n} = 0 & \text{on } \Gamma^0 \times ]0, T[. \end{array} \right.$$

*Proof.* We follow the Lagrangian method to prove the differentiability of  $J$ , this method gives a rapid derivation of  $J$  by introducing a Lagrangian function  $\mathcal{L}$  to separate the dependance of the state variables  $(c_1, c_2, c_3)$  and  $\Lambda = (\lambda_1, \lambda_2, \lambda_3)$ . We put by convention  $\lambda_0 = 0$  and we consider

$$\begin{aligned} \mathcal{L}(C, P, \Lambda, \sigma) &= \frac{1}{2} \sum_{i=1}^3 \int_0^T \int_{\Omega} (c_i - c_i^{obs})^2 d\sigma dt + \sum_{i=1}^3 \int_0^T \int_{\Omega} \left( \frac{\partial c_i}{\partial t} p_i + D \nabla c_i \nabla p_i \right) \\ &\quad + \sum_{i=1}^3 \int_0^T \int_{\Omega} \left( \nabla v \nabla p_i c_i + (\lambda_i c_i - \lambda_{i-1} c_{i-1}) p_i \right) + \sum_{i=1}^3 \int_{\Omega} \sigma_i (c_i(0) - c_i^0). \end{aligned}$$

For all  $(C, P, \Lambda, \sigma) \in L^2(0, T; H^1(\mathbb{R}^N))^3 \times L^2(0, T; H^1(\mathbb{R}^N))^3 \times [a, b]^3 \times L^2(\Omega)^3$ .

To obtain the initial boundary condition of the steady state, we derive the Lagrangian  $\mathcal{L}$  with respect to  $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ , for all  $\psi \in L^2(\Omega)$ , it follows that

$$\left\langle \frac{\partial \mathcal{L}}{\partial \sigma_i}, \psi \right\rangle = \int_{\Omega} \psi(c_i(0) - c_i^0)$$

for all  $\psi \in L^2(\Omega)$  the last integral vanishes if and only if  $c_i(0) = c_i^0$  in  $\Omega$ .

To get the adjoint equation we derive the Lagrangian with respect to the state variable  $(c_1, c_2, c_3)$ , for all  $\varphi \in L^2(0, T; H^1(\mathbb{R}^N))$ , one has

$$\begin{aligned} \left\langle \frac{\partial \mathcal{L}}{\partial c_1}, \varphi \right\rangle &= \int_0^T \int_{\Omega} \varphi(c_1 - c_1^{obs}) d\sigma dt + \int_0^T \int_{\Omega} \left( \frac{\partial \varphi}{\partial t} p_1 + D\nabla \varphi \nabla p_1 \right) \\ &\quad + \int_0^T \int_{\Omega} \left( \nabla v \nabla p_1 + \lambda_1 p_1 - \lambda_1 p_2 \right) \varphi + \int_{\Omega} \sigma_1 \varphi(0), \\ \left\langle \frac{\partial \mathcal{L}}{\partial c_2}, \varphi \right\rangle &= \int_0^T \int_{\Omega} \varphi(c_2 - c_2^{obs}) d\sigma dt + \int_0^T \int_{\Omega} \left( \frac{\partial \varphi}{\partial t} p_2 + D\nabla \varphi \nabla p_2 \right) \\ &\quad + \int_0^T \int_{\Omega} \left( \nabla v \nabla p_2 + \lambda_2 p_2 - \lambda_2 p_3 \right) \varphi + \int_{\Omega} \sigma_2 \varphi(0), \\ \left\langle \frac{\partial \mathcal{L}}{\partial c_3}, \varphi \right\rangle &= \int_0^T \int_{\Omega} \varphi(c_3 - c_3^{obs}) d\sigma dt + \int_0^T \int_{\Omega} \left( \frac{\partial \varphi}{\partial t} p_3 + D\nabla \varphi \nabla p_3 \right) \\ &\quad + \int_0^T \int_{\Omega} \left( \nabla v \nabla p_3 + \lambda_3 p_3 \right) \varphi + \int_{\Omega} \sigma_3 \varphi(0). \end{aligned}$$

We choose  $\sigma_i(x, y) = p_i(x, y, 0)$ , consequently the adjoint state is given as a solution  $P = (p_1, p_2, p_3)$  of the following problem

$$\left\{ \begin{array}{ll} -\frac{\partial p_1}{\partial t} = \nabla \cdot (D \cdot \nabla p_1) - \nabla p_1 \nabla v + \lambda_1 p_2 - \lambda_1 p_1 + c_1^{obs} - c_1 & \text{in } \Omega \times ]0, T[, \\ -\frac{\partial p_2}{\partial t} = \nabla \cdot (D \cdot \nabla p_2) - \nabla p_2 \nabla v + \lambda_2 p_3 - \lambda_2 p_2 + c_2^{obs} - c_2 & \text{in } \Omega \times ]0, T[, \\ -\frac{\partial p_3}{\partial t} = \nabla \cdot (D \cdot \nabla p_3) - \nabla p_3 \nabla v - \lambda_3 p_3 + c_3^{obs} - c_3 & \text{in } \Omega \times ]0, T[, \\ p_i(x, y, T) = 0 & \text{in } \Omega, i \in \{1, 2, 3\}, \\ D \frac{\partial p_i}{\partial n} = 0 & \text{on } \Gamma^0 \times ]0, T[. \end{array} \right. \quad (12)$$

To conclude the differentiability of  $J$ , we pass to derive the Lagrangian  $\mathcal{L}$  with respect to  $\Lambda = (\lambda_1, \lambda_2, \lambda_3)$ , we have

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \lambda_1} &= \int_0^T \int_{\Omega} c_1(p_1 - p_2), \\ \frac{\partial \mathcal{L}}{\partial \lambda_2} &= \int_0^T \int_{\Omega} c_2(p_2 - p_3), \\ \frac{\partial \mathcal{L}}{\partial \lambda_3} &= \int_0^T \int_{\Omega} c_3 p_3. \end{aligned}$$

Finally, we deduce the differentiability of  $J$  with respect to  $\lambda$ , moreover we have

$$\nabla J(\Lambda) = \left( \frac{\partial J(\Lambda)}{\partial \lambda_1}, \frac{\partial J(\Lambda)}{\partial \lambda_2}, \frac{\partial J(\Lambda)}{\partial \lambda_3} \right)$$

with  $(c_1, c_2, c_3)$  is solution of (4) and  $(p_1, p_2, p_3)$  is solution of the adjoint equation (12).  $\square$



## 5. PSOGSA algorithm

In this section we present the PSOGSA algorithm proposed by M. This algorithm is a hybridization of two meta heuristics. PSO proposed by Kennedy and Eberhart ([15][29]), and GSA proposed by E. Rashedi et al. [25].

We consider the following problem:

$$\min_{x \in \mathcal{D}} f(x) \quad (13)$$

where  $f$  is a function of  $\mathbb{R}^p$  with value in  $\mathbb{R}$  and  $\mathcal{D}$  a bounded subset of  $\mathbb{R}^p$ .

**5.1. PSO algorithm.** Particle Swarm Optimization (PSO) is an evolutionary algorithm inspired from social behavior of bird flocking. The principle is to generate a number of particles (possible solutions) which fly around in the search space to find best solution.

At each iteration, each particle in the population represents the current position in  $\mathcal{D}$  with the current velocity, it changes its velocity and position by considering the distance to pbest (personal best position) and the distance to gbest (global best) that can be modeled mathematically by:

$$v_i^{n+1} = wv_i^n + c_1 \times rand \times (pbest_i^n - x_i^n) + c_2 \times rand \times (gbest - x_i^n), \quad (14)$$

$$x_i^{n+1} = x_i^n + v_i^{n+1}, \quad (15)$$

with

- (1)  $v_i^n$  the velocity of the particle  $i$  at the  $n^{th}$  the iteration,
- (2)  $w$  the inertia weight,
- (3)  $c_1$  and  $c_2$  are the acceleration coefficients,
- (4)  $rand$  a random number between 0 and 1,
- (5)  $x_i^n$  the position of the particle  $i$  at the  $n^{th}$  iteration,
- (6)  $pbest_i^n$  the  $pbest$  of agent  $i$  at  $n^{th}$  iteration.

**5.2. GSA algorithm.** GSA is a heuristic optimization method proposed by E. Rashedi et al. [25]. This algorithm is inspired from the Newton's theory according to which "each particle particle in the universe attracts every other particle with a force that is directly proportional to the product of their masses and inversely proportional to the square of the distance between them". All masses attract each other by the gravitational forces between them.

In GSA, each mass has four characteristics: its position ( $X_i$ ), inertial mass ( $M_{ii}$ ), active gravitational mass ( $M_{ai}$ ), passive gravitational mass ( $M_{ip}$ ). The position of the mass in the search space represents a solution of the problem and its gravitational and inertial masses are determined using a fitness function of the problem.

Suppose a system with  $N$  agents in  $\mathcal{D}$ . The position of each agent is defined by:

$$X_i = (x_i^1, \dots, x_i^d, \dots, x_i^p), i = 1, 2, \dots, N. \quad (16)$$

According to Newton gravitation theory, the gravitational forces from agent  $j$  on agent  $i$  at the time  $t$  is defined as follow

$$F_{ij}^d = G(t) \frac{M_{pi(t)} \times M_{aj(t)}}{R_{ij}(t) + \varepsilon} (x_j^d(t) - x_i^d(t)), \quad (17)$$

where  $G(t)$  is gravitational constant at time  $t$ ,  $\varepsilon$  is a small constant, and  $R_{ij}(t)$  is the Euclidian distance between two agents  $i$  and  $j$ .  $G(t)$  is given by

$$G(t) = G_0 \times \exp(-\alpha \times \frac{iter}{Max_{iter}}), \quad (18)$$

where  $\alpha$  and  $G_0$  are descending coefficient and initial value respectively,  $iter$  is the current iteration, and  $Max_{iter}$  is maximum number of iterations.

The total force acting on agent  $i$  is calculated by the following formula

$$F_i^d(t) = \sum_{j=1, j \neq i}^N a_j \times F_{ij}^d(t), \quad (19)$$

where  $a_j$  is a random number in the interval  $[0,1]$ .

The acceleration  $\gamma_i^d$  of agent  $i$  is given by

$$\gamma_i^d(t) = \frac{F_i^d(t)}{M_{ii}(t)}. \quad (20)$$

Next velocity and position of agent  $i$  are calculated as follow:

$$v_i^d(t+1) = r_i \times v_i^d(t) + \gamma_i^d(t), \quad (21)$$

$$x_i^d(t+1) = x_i^d(t) + v_i^d(t+1), \quad (22)$$

where  $r_i$  is a random number in the interval  $[0,1]$ .

**5.3. PSO-GSA algorithm.** PSO-GSA proposed by Mirjalili et al (2017) [24] combine the ability of social thinking (*gbest*) in PSO with the local search capability of GSA. The velocity of agent  $i$  is given by

$$V_i(t+1) = w \times V_i(t) + c'_1 \times r_1 \gamma_i(t) + c'_2 \times r_2 \times (gbest - X_i(t)), \quad (23)$$

where  $V_i$  is the velocity of agent  $i$  at iteration  $t$ ,  $c'_1$  and  $c'_2$  are weighting factors,  $w$  is a weighting function,  $r_1$  and  $r_2$  are random numbers between 0 and 1,  $\gamma_i(t)$  is the acceleration of agent  $i$  at iteration  $t$ .

The position  $X_i$  ( $i = 1, \dots, N$ ), is given by

$$X_i(t+1) = X_i(t) + V_i(t+1). \quad (24)$$

**5.4. Algorithm.** In summary the resolution of our problem by PSO-GSA algorithm is given the algorithm below:

## 6. Results and discussions

The parameters of flow simulation are:

$D_m$	$\alpha_T$	$\alpha_L$	S	K	$\omega$
$10^{-7}$	0.01	0.1	0.02	0.001	0.33

TABLE 1. Parameters of flow.

---

```

Initialize the input parameters for PSO and GSA
Initialize the random position of search agents.
k ← 0
while k < Maxiter do
  for i=1 to N do
    Solving equation (1)
    Solving equation (4)
    Evaluate the score of each search agent using objective function (11)
    Update the G and gBest for each agent
    Calculate M, forces and accelerations for all agents
    Update velocity and position for each agent
  end for
  k ← k + 1
end while
Return the best solution
    
```

---

**6.1. Parameters identified.** Using our algorithm on the data above, we obtain the following results:

Parameters	Range	Identified values
$\lambda_1$	[0; 2]	0.06242
$\lambda_2$	[0; 2]	0.789
$\lambda_3$	[0; 3]	1.08

The Figure 3 shows a comparison between the level simulated and observed data. In analyzing this figure, we see that the concentration simulated coincide with the concentration observed.

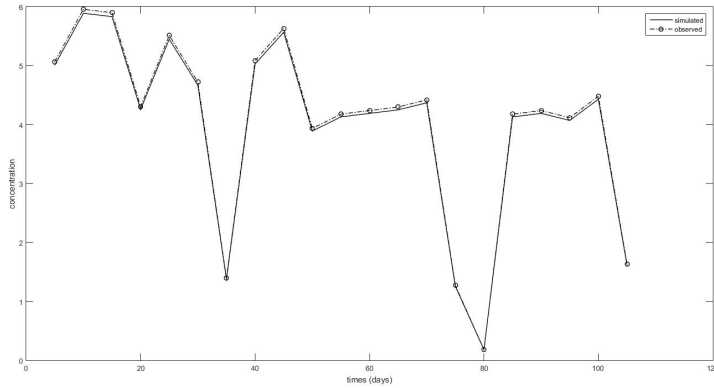


FIGURE 3. Curve of observed and simulated level to measurement dates.

**6.2. Spatial distribution of  $NH_4^-$  concentration.** The Figure 4 shows the removal rate of Nitrogen in the system. This rate increases at the beginning of the process to stabilize around 40% from the 30th day.

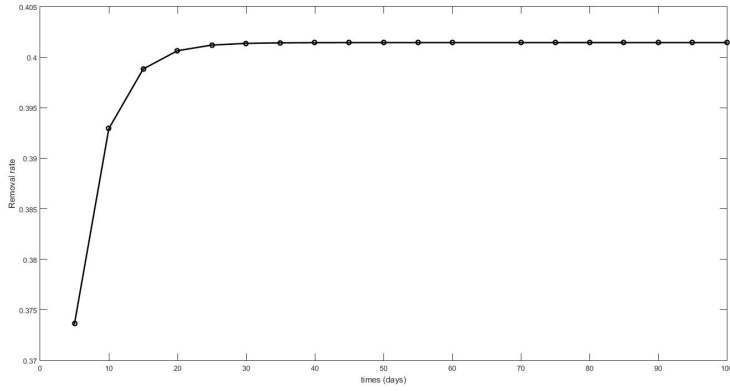


FIGURE 4. Curve of removal rate.

Figures 5 to 7 show spatial distribution of nitrogen in the system at different days respectively at 10, 50 and 100 days. As the case of the study on phosphorus in the [23], we note that concentrations vary considerably at the right and left borders of the system. They remain almost constant within the system.

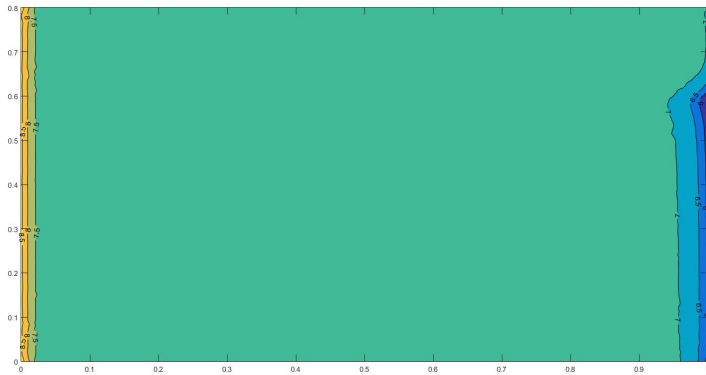


FIGURE 5. Day 10.

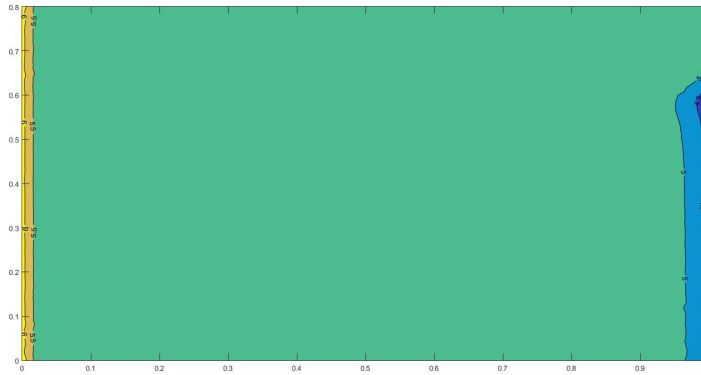


FIGURE 6. Day 50.

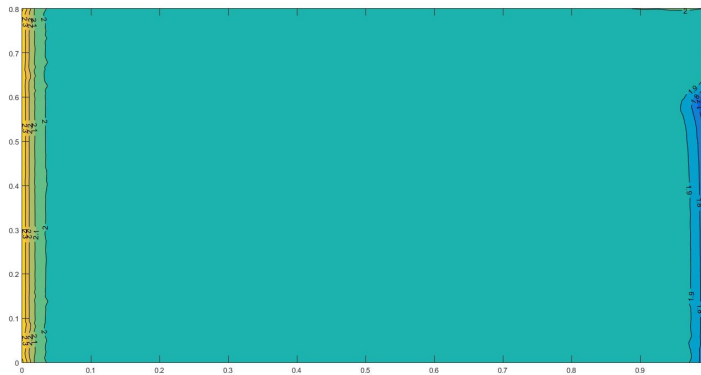


FIGURE 7. Day 100.

## 7. Conclusion

In this work, mathematical modeling and numerical simulation of hydrodynamics and nitrogen transformation processes in HSF constructed wetlands and porous media have been studied. The nitrogen kinetics has been modeled by hierarchical system of three advection dispersion-reaction equation. This system is solved by using the technique of operators splitting. The equation of advection is approximated by the Characteristics-Galerkin Method. The dispersion-reaction equation was carried by using the finite element method. The data used were measured in a bioreactor built in a primary school in Marrakech. Decay coefficient values, useful for design purposes, were determined by using Particle Swarm Optimization and Gravitational Search Algorithm (PSOGSA). The results of simulation show that the concentration of nitrogen simulated agrees fully with the one obtained by experimental data. The

removal rate of nitrogen in the system range between 37.5% and 40%.

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