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MODELING PLANT NUTRIENT UPTAKE: MATHEMATICAL ANALYSIS AND OPTIMAL CONTROL

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ABSTRACT. The article studies the nutrient transfer mechanism and its control for mixed cropping systems. It presents a mathematical analysis and optimal control of the absorbed nutrient concentration, governed by a transport-diffusion equation in a bounded domain near the root system, satisfying to the Michaelis-Menten uptake law.

The existence, uniqueness and positivity of a solution (the absorbed concentration) is proved. We also show that for a given plant we can determine the optimal amount of required nutrients for its growth. The characterization of the optimal control leading to the desired concentration at the root surface is obtained. Finally, some numerical simulations to evaluate the theoretical results are proposed.

1. Introduction. Plant nutrition has always been a main challenge in crop production but chemical fertilizers can be no longer the only sources of nutrients for crop growth and development. Switching from conventional intensive cropping systems to ecologically ones is necessary (see Griffon [6]). The awareness of the dependency to fossil fuels for the production of chemical inputs and the enactment of new rules for a healthier environment, have led to other agroecological alternatives in fertilizing practices. Plant growth is strongly linked to the amount of soil nutrients absorbed from its roots. These nutrients are produced naturally, they are present in the groundsoil at various levels of concentration. They may also be provided by humans in the form of chemical fertilizers, or by a secondary companion crop plants. It is the case for the nitrogen fixation and transfer from nitrogen fixing crops to cash crops in mixed cropping systems (see Jalonen et al. [8][9], Daudin and Sierra [3]).

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Modeling is required to understand the dynamics and the nutrient transfer mechanism and to define and test scenarios for the optimization of crop nutrition and sustainable systems. The root nutrient uptake as well as in solute movement in the soil are well explained by Tinker and Nye in [22], where they describe the uptake and nutrient motion processes from a biological and chemical point of view, and where they give the model of nutrient uptake and transfer using partial differential equations (PDE) known as the Nye-Tinker-Barber (NTB) system. Plant nutrition models that have emerged in the 60s with, among others, the works by Nye [14] and by Nye and Marriott [15]. See also the work by Itoh and Barber [7], or by Cushman [2] who suggests a general framework of the model of nutrient uptake by roots in which he adds a term called source or sink that models either the increase or the decrease in solute concentration w.r.t time and space.

More recently, Roose [19][20] used the NTB model in order to reflect in a more accurate way the morphology of the root system (modeling of root growth, root hair, mycorrhizae, ..) and the spatio-temporal dynamics of the solute in the soil. We also mention a recent work by Ptashnik [17], where the author studied a process of nutrient uptake by a single root branch using the asymptotic expansion method or a similar work by Schnepf et al. [21].

In the above mentioned works, no attempt was made concerning the question of optimal control for crop models. In this article we focus on the modeling of plant nutrient uptake by roots from multiple nutrient sources, and more precisely, on the determination of the optimal amount of nutrients that must be provided in the soil so that the plant grows in the best conditions to satisfy its demand.

This article is built as follows: in Section 2 we present the model of nutrient uptake and we provide a proof of existence and uniqueness of its solution. In Section 3, we study the optimal control question and we give a characterization of the optimal solution. Section 4 is devoted to some simulations where we compute the optimal nutrient input for a given plant’s growth in time.

2. Statement of the problem. Let \( \Omega \in \mathbb{R}^3 \) be the part of the soil close to the root called the rhizosphere, of regular boundary \( \Gamma = \Gamma_1 \cup \Gamma_2 \), such that \( \Gamma_1 \cap \Gamma_2 = \emptyset \) as shown in Figure 1. Here, \( \Gamma_1 \) represents the root surface and \( \Gamma_2 \) plays the role of the rhizosphere frontier to the rest of the soil. During a time \( t \in (0, T) \), the nutrient transport-diffusion and uptake by the roots is here described by the following Nye-Tinker-Barber (NTB) system:

\[
\begin{cases}
\frac{\partial c}{\partial t} + \mathbf{q} \cdot \nabla c - D \Delta c = 0 & \text{in } Q := [0, T] \times \Omega, \\
\text{div } \mathbf{q} = 0 & \text{in } Q, \\
\left( D \nabla c - \frac{1}{2} \mathbf{q} c \right) \cdot \mathbf{n} = \frac{I c}{K} & \text{on } \Sigma_1 := [0, T] \times \Gamma_1, \\
\left( D \nabla c - \frac{1}{2} \mathbf{q} c \right) \cdot \mathbf{n} = 0 & \text{on } \Sigma_2 := [0, T] \times \Gamma_2, \\
c(0, x) = c_0(x) & \text{in } \Omega,
\end{cases}
\]

where \( c = c(t, x) \) is the concentration of nutrient density at time \( t \) with position \( x \). The coefficient \( \alpha = b + \theta \) is a constant, where \( b \) is the buffer power and \( \theta \) the liquid saturation, the vector \( q = q(t, x) \) is the Darcy flux, and \( D \) the diffusion coefficient, which is a positive constant. The function \( h(c) = I c / K \) is the Michaelis-Menten function, and represents the inflow density to the root surface, where \( I \) is the maximum uptake constant, and \( K \) is the Michaelis-Menten constant.
2.1. Existence of a solution to the NTB problem. This part is devoted to
the weak formulation to problem (1) and to the proof of the existence of a positive
unique solution \( c(t, x) \). We will consider the function \( t \mapsto c(t, \cdot) \in V \) such that
\( V \subset H^1(\Omega) \). More precisely, consider the Hilbert space:
\[
V = \left\{ \psi \in H^1(\Omega) ; \psi|_{\Gamma_2} = 0 \right\},
\]
endowed with the \( H^1(\Omega) \) norm and equivalently with its semi-norm \( \| \nabla \psi \|_{L^2(\Omega)} \). We
also consider \( L^2(\Omega) \) as the pivot space i.e., \( V \subset \bar{L}^2(\Omega) \subset V' \).

Lemma 2.1. The problem (1) has the equivalent weak formulation given by the
following. Given \( c_0 \in V \), find \( c \in C([0, T]; V) \) such that:
\[
\begin{cases}
\frac{d}{dt} \int_{\Omega} c(t) \psi dx + a(t; c, \psi) = 0 \quad \forall \psi \in V, \\
c(0, x) = c_0(x),
\end{cases}
\]
where
\[
a(t; c, \psi) = \frac{1}{2} \int_{\Omega} q \cdot (\psi \nabla c - c \nabla \psi) \, dx + D \int_{\Omega} \nabla c \nabla \psi \, dx - \int_{\Gamma_1} I_c K \psi \, dx.
\]

Remark 1. We suppose that the concentration \( c(t, \cdot) \) belongs the set of continuous
functions in time \( c \in L^2([0, T]; V) \cap C([0, T]; L^2(\Omega)) \). The function \( c(t) \) is considered
as an element of \( V \) which represents the function \( x \mapsto c(t, x) \) for all \( t \in [0, T] \). We
point out that the regularity hypothesis on time is natural. The weak formulation
(2)-(3) is easy to get, and we refer to Allaire [1] or to Louison [13] for details.

Proposition 1 (Existence). We suppose that the flux \( q \) is uniformly bounded
\( q \in L^\infty(Q) \). Then, there is a unique solution \( c \in V \) to the problem (2)-(3).
Proof. We show first that the bilinear form \( a \) is continuous. We have by the Cauchy-
Schwartz inequality:
\[
|a(t; c, \psi)| \leq (q_\infty + D) ||c||_{V} ||\psi||_{V} + ||c||_{L^2(\Gamma_1)} ||\psi||_{L^2(\Gamma_1)}
\]
where \( q_\infty = ||q||_{L^\infty(Q)} \). Now since \( \varphi|_{\Gamma_2} = 0 \), for \( \varphi = c, \psi \), we have
\[
||\varphi||_{L^2(\Gamma_1)}^2 = 2 \int_{\Gamma_1} \varphi \nabla \varphi \, dx \leq 2 ||\varphi||_{L^2(\Omega)} ||\nabla \varphi||_{L^2(\Omega)} \leq 2 ||\varphi||^2_{V}.
\]
Hence, there is a positive constant $C > 0$ such that $|a(t;c,\psi)| \leq C\|c\|_{L^2} \|\psi\|_{L^2}$ with $C = q_\infty + D + 2$, which implies that $a$ is continuous.

Now we show that $a$ is coercive in the sense of evolution problems. We have:

$$a(t;c,c) = D \int_\Omega |\nabla c|^2 dx - \int_{\Gamma_1} \frac{I}{K} |c|^2 dx \geq D\|\nabla c\|^2_{L^2(\Omega)} - \|c\|^2_{L^2(\Gamma_1)}. \quad (4)$$

From the Young inequality we obtain $\|c\|^2_{L^2(\Gamma_1)} \leq \gamma\|c\|^2_{L^2(\Omega)} + \frac{1}{\gamma}\|\nabla c\|^2_{L^2(\Omega)}$. Hence, the bilinear form $a$ satisfies the conditions of J.-L. Lions’s Theorem (Cf. Lions-Magenes [12]), and we have Gårding’s inequality:

$$a(t;c,c) \geq \left(D - \frac{1}{\gamma}\right) \|c\|^2_{L^2} - \gamma\|c\|^2_{L^2(\Omega)} \quad \forall c \in V, \quad (5)$$

where $\gamma$ is a positive constant chosen such that we have $\gamma D > 1$. The hypothesis of the Lions theorem are then satisfied, and (1) has a unique weak solution $c \in V$. \qed

2.2. **Positivity of the solution.** As usual, we denote by $c = c^+ - c^-$, for the solution $c \in V$, where $c^+$ and $c^-$ are the classical nonnegative parts of $c$. We have the following result:

**Lemma 2.2 (Positivity).** Let be $c = c(x,t)$ the solution to the NTB system. Suppose that $c_0 \geq 0$ and that $c_{\Sigma_1} \geq 0$, then $c$ is non-negative and we have:

$$c(T,.) \geq 0, \quad \forall T > 0.$$

**Proof.** We will show that $c^- = 0$. We multiply the NTB system by $c^-$ and we integrate by parts over $Q$. Since $(\partial_t c^+)c^- = (\nabla c^+)c^- = (\Delta c^+)c^- = 0$, we have for each integral:

$$-\alpha \int_0^T \int_\Omega (\frac{\partial c^-}{\partial t}) c^- dx dt = -\frac{\alpha}{2} \left( \int_\Omega |c^- (T)|^2 - |c^- (0)|^2 dx \right),$$

and with the Gauss formula $\text{div} \; q = 0$ in $\Omega$,

$$-\int_\Omega (q \cdot \nabla c^-) c^- dx dt = -\int_0^T \frac{1}{2} \int_\Gamma (q.e^-) c^- n dx dt,$$

and,

$$D \int_Q (\Delta c^-) c^- dx dt = D \int_\Sigma (\nabla c^-) c^- n dx dt - D \int_Q |\nabla c^-|^2 dx dt.$$ 

thanks to the Green formula. Adding the three integrals we find:

$$-\frac{\alpha}{2} \left( \int_\Omega |c^- (T)|^2 - |c^- (0)|^2 dx \right) + \int_\Gamma \frac{I}{K} \|c^-\|^2 n dx dt = D \int_Q |\nabla c^-|^2 dx dt \geq 0.$$

Now since $c^-_{\Sigma_1} = 0$ we obtain $\|c^- (T)\|_{L^2(\Omega)} \leq \|c^- (0)\|_{L^2(\Omega)} = 0, \quad \forall T \geq 0. \quad \Box$

3. **Optimal control for the NTB model.** We here study the optimal control for the NTB system (1). Nutrients come from the second plant by exudates through $\Gamma_2$, and there, we put a control function. First, we rewrite the NTB system using simple notations:

$$\begin{align*}
A c &= 0 \quad \text{in} \quad Q := ]0,T[ \times \Omega, \\
B c.n &= \frac{I}{K} c \quad \text{on} \quad \Sigma_1 := ]0,T[ \times \Gamma_1, \\
B c.n &= w \quad \text{on} \quad \Sigma_2 := ]0,T[ \times \Gamma_2, \\
c(0,x) &= 0 \quad \text{in} \quad \Omega, 
\end{align*} \quad (6)$$
where we have:

$$A = \alpha \frac{\partial}{\partial t} + q \nabla - D \Delta, \quad \text{and} \quad B = D \nabla - \frac{1}{2} q.$$

Here, \( w = -v \) where \( v \) is a positive control function. It corresponds to the addition of nutrient in the soil. It is prescribed in the rhizosphere frontier \( \Gamma_2 \) as an inflow nutrient.

The existence of a solution to (6) can be deduced from the one of Proposition 1, since we have:

**Corollary 1.** Under the hypothesis of Proposition 1, we suppose that \( w \in L^2(\Sigma_2) \). Then, there is a unique solution \( c \in V \) to the weak problem (2) with \( c_0 = 0 \), and with \( a(t; c, \psi) \) in (5) replaced by:

$$b(t; c, \psi) = a(t; c, \psi) - \int_{\Gamma_2} w \psi \, dx, \quad \psi \in V. \quad (7)$$

The goal in this paper is to characterize the control which minimizes the cost function:

$$J(v) = \|c(v) - \bar{c}\|_{L^2(\Sigma_1)}^2 + N\|v\|_{L^2(\Sigma_2)}^2, \quad (8)$$

where \( \bar{c} \) is the observation given for \( L^2(\Sigma_1) \), and where \( N > 0 \) is a positive constant. The control function \( v \) is taken in the region \( L^2(\Sigma_2) \) of \( \Omega \). The control problem is similar to a regional control problem as introduced by El Jai et al. [4], and El Jai [5] for example.

### 3.1. Existence of the optimal control.

**Proposition 2.** There exists a unique \( u \in U = L^2(\Sigma_2) \) such that

$$J(u) = \inf_{v \in U} J(v).$$

**Proof.** The existence of the control is easy to prove since the \( L^2 \) norm in \( J \) is continuous and coercive. Moreover, we have

$$J(v) \geq J(0) = 0, \quad \forall v \in L^2(\Sigma_2),$$

hence there exists a positive constant \( m > 0 \) such that \( m = \inf_{v \in L^2(\Sigma_2)} J(v) \).

Let \( v_n \) be a minimizing sequence satisfying \( m = \lim_{n \to \infty} J(v_n) \). For every \( n \in \mathbb{N}, n > n_0 \),

$$J(0) \leq J(v_n) \leq m + 1.$$

Hence, there exists a constant \( d \geq \sqrt{m + 1} \) independent of \( n \) such that

$$\|v_n\|_{L^2(\Sigma_2)} \leq d, \quad \text{and} \quad \|c(v_n)\|_{L^2(\Sigma_1)} \leq d.$$

Therefore \( v_n \rightharpoonup u \in L^2(\Sigma_2) \) weakly, and \( c(v_n) \rightharpoonup c(u) \) weakly in \( L^2(\Sigma_1) \) because \( c \) is a continuous function.

Finally, we deduce from the strict convexity of the cost function \( J \) that \( u \) is unique. \( \square \)
3.2. Characterization of the optimal control. We give a first characterization of the optimal control \( u \in L^2(\Sigma_2) \) in the following lemma:

**Lemma 3.1.** The optimal control \( u \) of the problem (6)-(8) satisfies to:

\[
\int_{\Sigma_1} (c(u) - \tilde{c}) c(w) \cdot n \, dx dt + N \int_{\Sigma_2} uw \cdot n \, dx dt = 0, \quad \forall w \in L^2(\Sigma_2).
\]

**Proof.** We have the Euler-Lagrange equality satisfied by the optimal control \( u \):

\[
\lim_{\lambda \to 0} \left( \frac{J(u + \lambda w) - J(u)}{\lambda} \right) = 0, \quad \forall w \in L^2(\Sigma_2).
\]

Then

\[
\frac{J(u + \lambda w) - J(u)}{\lambda} = \lambda ||c(w)||_{L^2(\Sigma_1)}^2 + 2\lambda (c(u) - \tilde{c}, c(w))_{L^2(\Sigma_1)} + 2N (u, w)_{L^2(\Sigma_2)} + \lambda N ||w||_{L^2(\Sigma_2)}^2.
\]

Hence,

\[
\lim_{\lambda \to 0} \left( \frac{J(u + \lambda w) - J(u)}{\lambda} \right) = 2(c(u) - \tilde{c}, c(w))_{L^2(\Sigma_1)} + 2N (u, w)_{L^2(\Sigma_2)} = 0,
\]

which is the desired equality (9).

\[
\begin{align*}
\text{Figure 2.} \quad & \text{The Michaelis-Menten uptake function } h(c) = \frac{Ic}{K} \text{ prescribed on the root surface } \Gamma_1. \text{ The boundary control } u(t,x), \text{ which represents an addition of nutrient into the rhizosphere region is prescribed on } \Gamma_2. \\
\end{align*}
\]

Now, we give the optimality system (SO) for the optimal control \( u \). We have the following theorem:

**Theorem 3.2** (Optimality system). The optimal control \( u \) for the problem (6)-(8) is characterized by the triplet \( \{ u, c(u), p(u) \} \) solution to the optimality system:

\[
\begin{cases}
Ac = 0 \quad & A^*p = 0 \quad \text{in } Q, \\
Bc \cdot n = \frac{I}{K}c \quad & B^*p \cdot n = c(u) - \tilde{c} + \frac{I}{K}p \quad \text{on } \Sigma_1, \\
Bc \cdot n = -u \quad & B^*p \cdot n = 0 \quad \text{on } \Sigma_2, \\
c(0,x) = 0 \quad & p(T,x) = 0 \quad \text{in } \Omega,
\end{cases}
\]

and by the adjoint equation:

\[
p + Nu = 0 \in L^2(\Sigma_2).
\]
Proof. We introduce the function \( p = p(t, x) \) solution to the adjoint problem :

\[
\begin{cases}
A^* p = 0 & \text{in } Q, \\
B^* p \cdot n = c(u) - \tilde{c} + \frac{I}{K} p & \text{on } \Sigma_1, \\
B^* p \cdot n = 0 & \text{on } \Sigma_2, \\
p(T, x) = 0 & \text{in } \Omega.
\end{cases}
\]

(13)

where

\[
A^* = -\alpha \frac{\partial}{\partial t} - q \cdot \nabla - D \Delta, \quad B^* = -D \nabla - \frac{1}{2} q.
\]

We multiply the first equation of (13) by \( c(w) \), and we integrate by parts over \( Q \). We first have :

\[
-\alpha \int_Q \left( \frac{\partial p}{\partial t} \right) c(w) \, dx \, dt = \alpha \int_Q \left( \frac{\partial c}{\partial t} \right)(w) \, p \, dx \, dt.
\]

(14)

With the Gauss property we have \( q \cdot \nabla p = \text{div}(q p) - p \text{div} q = \text{div}(q p) \). We integrate over \( x \), we have on one hand :

\[
\int_Q (q \cdot \nabla p) c(w) \, dx \, dt = \int_Q \text{div}(q p) c(w) \, dx \, dt
\]

\[
= \int_Q \left( \text{div}(q p c(w)) - q p \cdot \nabla c(w) \right) \, dx \, dt
\]

\[
= \int_\Sigma q p c(w) n \, dx \, dt - \int_Q q p \cdot \nabla c(w) \, dx \, dt
\]

(15)

using the Gauss theorem. On the other hand, using the Green formula we have :

\[
-\int_Q (D \Delta p) c(w) \, dx \, dt = -\int_\Sigma (D \nabla p) c(w) \cdot n \, dx \, dt + \int_\Sigma (D \nabla c(w)) p \cdot n \, dx \, dt
\]

\[
- \int_Q (D \Delta c(w)) p \, dx \, dt.
\]

We resume by

\[
0 = \int_Q \left( A^* p \right) c(w) \, dx \, dt
\]

\[
= \int_Q \left( \alpha \frac{\partial c(w)}{\partial t} + q \cdot \nabla c(w) - D \Delta c(w) \right) p \, dx \, dt
\]

\[
- \int_\Sigma \left( D \nabla p + \frac{1}{2} q p \right) c(w) \cdot n \, dx \, dt + \int_\Sigma \left( D \nabla c(w) - \frac{1}{2} q c(w) \right) p \cdot n \, dx \, dt
\]

\[
= -\int_{\Sigma_1} \left( \tilde{c} - c(u) + \frac{I}{K} p \right) c(w) \cdot n \, dx \, dt + \int_{\Sigma_1} \frac{I}{K} c(w) p \cdot n \, dx \, dt
\]

\[
- \int_{\Sigma_2} w p \cdot n \, dx \, dt
\]

\[
= -\int_{\Sigma_1} \left( \tilde{c} - c(u) \right) c(w) \cdot n \, dx \, dt - \int_{\Sigma_2} w p \cdot n \, dx \, dt.
\]

Hence,

\[
(c(u) - \tilde{c}, c(w))_{L^2(\Sigma_1)} = \langle w, p \rangle_{L^2(\Sigma_2)}.
\]

(16)

Replacing in (9), we finally have :

\[
\langle p + N u, w \rangle_{L^2(\Sigma_2)} = 0, \quad \forall \, w \in L^2(\Sigma_2).
\]
4. Numerical results. To ease reader’s reading and understanding in the interpretation of the below results we make the computations in one dimension of space. In this situation the spatial motion of nutrients is produced along an horizontal axis $[x_0,x_{N_x+1}]$ on which the point at the right extrema corresponds to the uptake point at the root surface ($\Gamma_1 = x_{N_x+1}$) and the point at the left extrema corresponds to the input point of nutrients ($\Gamma_2 = x_0$). In this case the optimal control problem is written by

$$
[P] = \begin{cases} 
\min_{v \in L^2(\Sigma_2)} & J(v) \\
\text{where} & J(v) = \int_0^T [c(t,x_{N_x+1}) - \hat{c}(t,x_{N_x+1})]^2 dt + \frac{N \|v\|_{L^2(\Sigma_2)}^2}{\sqrt{|x_{N_x+1} - x_0|}} \\
\text{and where } c \text{ satisfies the nutrient uptake model } (6), & \text{with } \Sigma_1 = (0,T) \times \{x_{N_x+1}\} \text{ and } \Sigma_2 = (0,T) \times \{x_0\}.
\end{cases}
$$

The function $\hat{c}$ is a given nutrient uptake dynamics at the root surface and $v$ is the searching control that solve the problem $[P]$.

The optimal control problem $[P]$ is numerically solved by a Quasi-Newton method whose the algorithm is available on Matlab tools or on Absoft software (see Picart and Ainseba [16] who used the method for hyperbolic systems). Here we used the latter with the BCONF routine which is well adapted for our problem. The solution of NTB-system is numerically computed with a Difference Element scheme of Euler kind that is reported in Annex. The parameters of the NTB-system are chosen so that a spatial motion is observed on the time and space domain $(0,5) \times [0,1]$ that is

$$q = 0.5, \quad D = 0.1, \quad \alpha = 1, \quad I = 0.001, \quad K = 1,$$

with a space-discretization step equal to 0.1, and a time-discretization step equal to 0.01.

We numerically test our problem with the function $\hat{c}$ of Figure 3. The root nutrient uptake is like a sigmoid curve that increases with time until to reach a maximum nutrient uptake value of 2.8. The function $\hat{c}$ is obtained by solving NTB-system with a given control function that is represented in dotted curve on Figure 4 and called exact control function. The input of nutrients is a step-function equal to one during the first 4 units of time and to 0 after that. The numerical result consists in finding for this given nutrient uptake dynamics $\hat{c}$ the optimal control solution of problem $[P]$ that allows to reach it. For this, we initialize the Quasi-Newton algorithm with the step-function represented by the double-dotted curve of Figure 4. The optimal control solution is then obtained when the value of the cost function $J(v)$ at the optimal control solution is close to zero.

The optimal solution is given by the solid curve of Figure 4. The $L^2$-error of the difference between the estimated solution and the exact one (dotted curve) is of order $1.5910^{-3}$ meaning that the QN’s algorithm has converged toward the exact solution. In this example the numerical optimal solution is unique.

We conclude this work by a final remark:

**Remark 2.** In this paper we proposed a model of nutrient uptake by roots whose origin is either the soil or root exudates from a secondary plant [6]. This model
Figure 3. Nutrient uptake at the root surface with respect to time. This curve is used to define the $\tilde{c}$ function in problem $[P]$. 

Figure 4. Nutrient input from exudates with respect to time. The dotted curve is the control function used to construct the function $\tilde{c}$ by solving the NTB-system. The double dotted curve is the initial control used in the Quasi-Newton algorithm. The solid curve is the numerical solution of $[P]$. 
derives from the NTB model which describes the transport and diffusion of nutrients through the soil to the root surface in general. These initial theoretical and numerical results are encouraging for the study and development of alternative methods to fertilizing plants through the soil or the contribution of service plants for example.

5. **Annex.** Let $\Omega = [x_1, x_{N_x}]$ be the domain of the space variable, with $N_x$ the space-point number. Let $x_i = i\Delta x$ be the space discretization point, for $i = 1, N_x$, with $\Delta x$ the space discretization step. The time discretization point is defined by $t^n = n\Delta t$, with $n \geq 0$ and $\Delta t$ the time discretization step. The numerical solution of the NTB-system of (6) is given by the following scheme

$$\frac{c^{n+1}_i - c^n_i}{\Delta t} = F(c^n_i, x_i, t^n),$$

for $i$ from 1 to $N_x$ and $n \geq 0$, where

$$F(c^n_i, x_i, t^n) = -\frac{q}{\alpha} c^n_i - \frac{D c^{n+1}_i - 2c^n_i + c^{n-1}_i}{\Delta x^2}.$$ 

We get a system of equations that can be rewritten as the following matrix form

$$C^{n+1} = \frac{\Delta t}{\alpha} AC^n,$$

where $A$ is given by

$$A = \begin{bmatrix}
\frac{\alpha}{\Delta t} - \frac{q}{\Delta x} - \frac{2D}{\Delta x^2} & \frac{D}{\Delta x^2} & \cdots & 0 \\
\frac{q}{\Delta x} + \frac{D}{\Delta x^2} & \frac{\alpha}{\Delta t} - \frac{q}{\Delta x} - \frac{2D}{\Delta x^2} & \cdots & 0 \\
0 & \frac{q}{\Delta x} + \frac{D}{\Delta x^2} & \frac{\alpha}{\Delta t} - \frac{q}{\Delta x} - \frac{2D}{\Delta x^2} & \cdots \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
0 & \cdots & \frac{q}{\Delta x} + \frac{D}{\Delta x^2} & \frac{\alpha}{\Delta t} - \frac{q}{\Delta x} - \frac{2D}{\Delta x^2} 
\end{bmatrix}.$$ 

The boundary conditions at the point $x_0$ and $x_{N_x+1}$ are respectively approximated by

$$c^n_{x_0} = c^n_2 + \Delta x \left( v^n - \frac{q}{2} c^n_1 \right),$$

$$c^n_{x_{N_x+1}} = c^n_{x_{N_x-1}} + \Delta x \left( h^n_{N_x} + \frac{q}{2} c^n_{N_x} \right),$$

for all time $n \geq 0$.

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