

## Analysis of a model of phosphorus uptake by plant roots

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*Abstract.* In this paper, we consider a model of phosphorus uptake by plant roots, governed by a quasilinear parabolic equation. We first study the well posedness of the associated Cauchy problem. Then, we consider a shape optimization problem: how to deform the shape of the root in order to increase phosphorus uptake. Finally, we give some numerical results of the shape optimization process.

### 1. Introduction

Phosphorus (P) is an essential element for plant growth and metabolism. It is involved in many plant processes such as energy transfer, the synthesis of nucleic acids and membranes, plant respiration, photosynthesis and enzyme regulation. Adequate phosphorus nutrition stimulates early plant growth and hastens maturity.

Phosphorus (P) is one of the limiting factors for plant growth in many agricultural systems. P uptake by plants is often constrained by the very low solubility of P in the soil, as P is mostly present in unavailable forms because of adsorption, precipitation or conversion to the organic form.

This leads to the application of up to four times the fertilizer necessary for crop production. This practice can result in polluted water systems, imbalanced ecosystems and degradation of the environment. Moreover, at the current rate of usage of P fertilizer, readily available sources of phosphate rocks could be depleted in as little as 60–90 years.

This brings us to consider the problem of reducing fertilizer usage of P, which suggests improved efficiency of fertilizer methods in the short term and adaptation of genotypes to P-deficient soils in the long term.

We therefore propose to study the transfer of P in the soil as well as its uptake by plant roots, as was done by [2, 10] and [9]. P moves in soil through both diffusion and mass flow, although diffusion is dominant.

Let us consider a shape modeling the root surface. The exterior domain around the root is the studied section of the soil. Let us denote by  $\Omega \subset \mathbb{R}^d$  ( $d = 2, 3$ ) the soil

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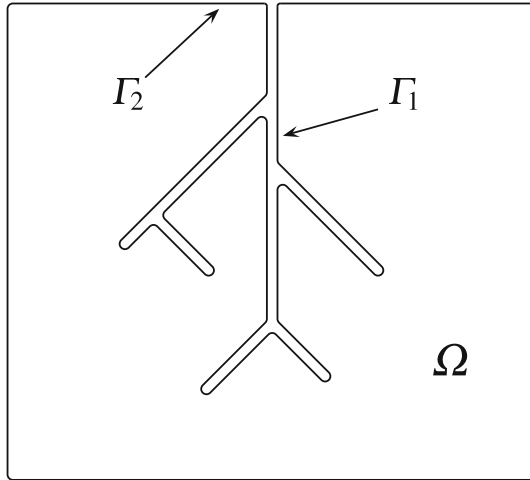


Figure 1. Configuration of the domain

domain, delimited by the root surface and the domain boundaries. Let  $\Gamma = \partial\Omega$ . Let  $\Gamma_1$  be the boundary representing the root surface and  $\Gamma_2 = \Gamma \setminus \Gamma_1$  (Fig. 1).

Let  $T > 0$  be given and  $I = [0, T]$ . The evolution of the concentration  $c$  of P in the soil is governed by the following convection–diffusion equation:

$$\begin{cases} \partial_t(\theta c + \varphi(c)) = \operatorname{div}(A\nabla c - \mathbf{q}c) - R & \text{in } I \times \Omega, \\ \alpha h(c) = -(A\nabla c - \mathbf{q}c) \cdot \mathbf{n} & \text{on } I \times \Gamma_1, \\ 0 = (A\nabla c - \mathbf{q}c) \cdot \mathbf{n} & \text{on } I \times \Gamma_2, \\ c(0, x) = c^0(x) & \text{in } \Omega, \end{cases} \quad (1.1)$$

where

- $\mathbf{n}$  is the unit outward normal to the boundary of the domain,
- $c^0$  is the initial P concentration,
- $A$  is the diffusion coefficient of P in the soil,
- $\theta$  is the volumetric water content,
- $\mathbf{q}$  is the groundwater flow,
- $\varphi$  is an adsorption/desorption isotherm relating the amount of adsorbed P to the equilibrium concentration of P in solution; an example is the Freundlich adsorption isotherm [8], defined by:

$$\varphi(c) = \kappa c^b \quad \text{for } c \in [0, +\infty), \quad \kappa > 0, \quad b \in (0, 1),$$

- $h$  is a model of enzyme kinetics, relating in this case the root uptake rate of P to its concentration at the root surface; an example is the Michaelis–Menten model [1], given by:

$$h(c) = \frac{F_m c}{K_m + c} \quad \text{for } c \in [0, +\infty), \quad F_m > 0, \quad K_m > 0,$$

- $R$  represents additional optional source/sink terms to the system. We will only consider source terms, such as fertilizer application,
- $\alpha$  is a parameter we introduce in order to obtain sufficient regularity of the boundary condition in the case  $\Gamma_1 \cap \Gamma_2 \neq \emptyset$ :  $\alpha \in C^\infty(\mathbb{R}^d)$  such that for  $x \in \Gamma$

$$\begin{cases} 0 \leq \alpha(x) \leq 1 & \text{on } \Gamma_1 \\ \alpha(x) = 0 & \text{on } \Gamma_2. \end{cases}$$

We do not restrict ourselves to considering explicit forms for  $\varphi$  or  $h$ : we only use general properties of these functions throughout this paper.

Since  $\varphi$  is defined on  $[0, +\infty[$ , we consider positive solutions of problem (1.1).

The paper is organized as follows: We first discuss existence and uniqueness of solutions to problem (1.1).

Then, we introduce a shape optimization method which enables us to modify the shape of the domain in order to maximize the amount of absorbed P, represented by the shape functional

$$J(c) = \int_0^T \int_{\Gamma_1} h(c),$$

subject to the volume constraint  $|\Omega| = \text{constant}$ .

Finally, we give a numerical example of the shape optimization process in two spatial dimensions.

## 2. A priori estimates

In this section, we derive upper and lower bounds for the solutions of problem (1.1) in the space  $C^{1,2}(\overline{Q})$ .

Let us first introduce some notations:

- $S$  is the boundary of  $\Omega$ ,
- $Q$  is the cylinder  $(0, T) \times \Omega$ ,
- $S_T$  is the lateral surface of  $Q$ :  $S_T = \{(t, x) \mid t \in [0, T], x \in S\}$ ,
- $\theta^0(x) := \theta(0, x)$  for  $x \in \overline{\Omega}$ .

Moreover, we make the following assumptions:

hypotheses on  $S$

$$S \in C^{2+\beta}, \tag{2.1}$$

hypotheses on  $c^0$

$$\begin{aligned} c^0 &\in C^{2+\beta}(\overline{\Omega}), \quad c^0 > 0, \\ (A \nabla c^0 - \mathbf{q}c^0) \cdot \mathbf{n} + h(c^0) &= 0 \quad \text{on } \Gamma_1, \\ (A \nabla c^0 - \mathbf{q}c^0) \cdot \mathbf{n} &= 0 \quad \text{on } \Gamma_2, \end{aligned} \tag{2.2}$$

hypotheses on  $\varphi$

$$\varphi \in C^3((0, +\infty)), \quad \varphi' > 0, \tag{2.3}$$

hypotheses on  $A$

$$A \in C^{1+\beta/2, 2+\beta}(\overline{Q}), \quad A_m \geq A(t, x) \geq A_0 > 0 \quad \text{in } \overline{Q}, \tag{2.4}$$

hypotheses on  $\theta$

$$\theta \in C^{1+\beta/2, 2+\beta}(\overline{Q}), \quad \theta_m \geq \theta(t, x) \geq \theta_0 > 0 \quad \text{in } \overline{Q}, \tag{2.5}$$

hypotheses on  $R$

$$R \in C^{1+\beta/2, 2+\beta}(\overline{Q}), \quad R < 0 \quad \text{in } \overline{Q}, \tag{2.6}$$

hypotheses on  $\mathbf{q}$

$$q_i \in C^{1+\beta/2, 2+\beta}(\overline{Q}), \quad i = 1, \dots, d, \tag{2.7}$$

let us extend  $h$  to  $\mathbb{R}$  so that

$$h \in C^2(\mathbb{R}), \quad h(0) = 0, \quad \|h\|_{L^\infty(\mathbb{R})} + \|h'\|_{L^\infty(\mathbb{R})} + \|h''\|_{L^\infty(\mathbb{R})} \leq C_h. \tag{2.8}$$

Here and in the sequel,

$$\beta \in (0, 1). \tag{2.9}$$

Now, let  $c$  be a solution of problem (1.1) in the space  $C^{1,2}(\overline{Q})$ ,  $c \geq 0$  in  $\overline{Q}$ .

- Estimate from below:

Let  $\varepsilon > 0$ , and let  $T' = \max\{t \in [0, T] \mid c \geq \varepsilon \text{ in } [0, T'] \times \overline{\Omega}\}$ .

We now find a lower bound for  $c$  in  $[0, T'] \times \Omega$ .

Let us introduce the following function

$$\hat{c}(t, x) := \delta e^{-Kt} \hat{c}_0(x), \quad (t, x) \in Q, \tag{2.10}$$

where  $\delta, K > 0$  are chosen below and where  $\hat{c}_0 \in C^2(\overline{\Omega})$  is a strictly positive function satisfying

$$A_0 \frac{\partial \hat{c}_0}{\partial n} < -\|\mathbf{q}\|_{L^\infty(Q)} \hat{c}_0(x) - (h'(0) + 1) \hat{c}_0(x) \quad \forall x \in S, \tag{2.11}$$

and

$$0 < \hat{c}_0(x) < 1 \quad \forall x \in \overline{\Omega}. \tag{2.12}$$

Choosing now  $K$  large enough and  $\delta$  small enough,  $\hat{c}$  satisfies

$$\begin{cases} \theta \hat{c}_t - \operatorname{div}(A \nabla \hat{c} - \mathbf{q} \hat{c}) + R + \theta_t \hat{c} < 0 & \text{in } Q, \\ A \frac{\partial \hat{c}}{\partial n} < (\mathbf{q} \cdot \mathbf{n}) \hat{c} - \alpha h(\hat{c}) & \text{on } S_T, \\ \hat{c}(0, x) < c^0(x) & \text{in } \overline{\Omega}. \end{cases} \tag{2.13}$$

Since  $\varphi' \geq 0$ , we can see that

$$(\theta + \varphi'(\hat{c}))\hat{c}_t - \operatorname{div}(A\nabla\hat{c} - \mathbf{q}\hat{c}) + R + \theta_t\hat{c} < 0 \quad \text{in } Q. \tag{2.14}$$

We now apply a comparison principle which results from the following theorem:

**THEOREM 1.** ([3, Theorem 17 p. 53]) *Let  $v$  and  $w$  be two continuous functions in  $\overline{Q}$ , and let the first  $t$ -derivative and the first two  $x$ -derivatives of  $v, w$  be continuous in  $\overline{Q}$ . Let  $F(t, x, p, p_i, p_{ij})$  ( $i, j = 1, \dots, d$ ) be a continuous function together with its first derivatives with respect to the  $p_{hk}$  in a domain  $E$  containing the closure of the set of points  $(t, x, p, p_i, p_{ij})$  where*

$$(t, x) \in Q, \quad p \in (v(t, x), w(t, x)), \quad p_i \in \left( \frac{\partial v(t, x)}{\partial x_i}, \frac{\partial w(t, x)}{\partial x_i} \right),$$

$$p_{ij} \in \left( \frac{\partial^2 v(t, x)}{\partial x_i \partial x_j}, \frac{\partial^2 w(t, x)}{\partial x_i \partial x_j} \right);$$

here  $(a, b)$  denotes the interval connecting  $a$  to  $b$ . Assume also that  $(\partial F / \partial p_{hk})$  is a positive semidefinite matrix.

If

$$\begin{cases} \frac{\partial v}{\partial t} > F\left(t, x, v, \frac{\partial v}{\partial x_i}, \frac{\partial^2 v}{\partial x_i \partial x_j}\right) & \text{in } Q, \\ \frac{\partial w}{\partial t} \leq F\left(t, x, w, \frac{\partial w}{\partial x_i}, \frac{\partial^2 w}{\partial x_i \partial x_j}\right) & \text{in } Q, \\ v(0, x) > w(0, x) & \text{on } \overline{\Omega}, \\ \frac{\partial v}{\partial n} + \gamma(t, x, v) > \frac{\partial w}{\partial n} + \gamma(t, x, w) & \text{on } S_T, \end{cases} \tag{2.15}$$

for some function  $\gamma$ , then also  $v > w$  in  $Q$ .

We have

$$\begin{cases} c_t = (\theta + \varphi'(c))^{-1}(\operatorname{div}(A\nabla c - \mathbf{q}c) - R) - \theta_t c & \text{in } [0, T'] \times \Omega, \\ A\nabla c \cdot \mathbf{n} = (\mathbf{q} \cdot \mathbf{n})c - \alpha h(c) & \text{on } [0, T'] \times S, \end{cases} \tag{2.16}$$

and

$$\begin{cases} \hat{c}_t < (\theta + \varphi'(\hat{c}))^{-1}(\operatorname{div}(A\nabla\hat{c} - \mathbf{q}\hat{c}) - R) - \theta_t\hat{c} & \text{in } [0, T'] \times \Omega, \\ A\nabla\hat{c} \cdot \mathbf{n} < (\mathbf{q} \cdot \mathbf{n})\hat{c} - \alpha h(\hat{c}) & \text{on } [0, T'] \times S. \end{cases} \tag{2.17}$$

Moreover,  $\hat{c}(0, x) < c(0, x)$  in  $\overline{\Omega}$ .

It is easy to see that in our case,  $F$  satisfies the hypotheses of Theorem 1 thanks to (2.3), (2.4), (2.5), (2.6) and (2.7).

Thus, we can apply Theorem 1 to  $c$  and  $\hat{c}$  in  $[0, T'] \times \Omega$  in order to deduce that

$$c > \hat{c} \geq \delta e^{-KT} \min_{x \in \overline{\Omega}} \hat{c}_0(x) > 0 \quad \text{in } [0, T'] \times \Omega. \tag{2.18}$$

We proved that for every  $\varepsilon > 0$ , we have  $c > \delta e^{-KT} \min_{x \in \overline{\Omega}} \hat{c}_0(x)$  in  $[0, T'] \times \Omega$ , with  $T' = \max\{t \in [0, T] \mid c \geq \varepsilon \text{ in } [0, T'] \times \overline{\Omega}\}$ . Note that the lower bound is

independent of the choice of  $\varepsilon$ . Then, it is easy to see that if we take  $\varepsilon$  small enough and we suppose that  $T' < T$ , by a continuity argument ( $c \in C^{1,2}(\overline{Q})$ ) we obtain that  $c \geq \varepsilon$  in  $[0, T' + \delta t] \times \overline{\Omega}$  for some  $\delta t > 0$ , which leads to a contradiction. Thus,  $T' = T$  and we can conclude that

$$c > \delta e^{-KT} \min_{x \in \overline{\Omega}} \hat{c}_0(x) > 0 \quad \text{in } Q. \tag{2.19}$$

- Estimate from above:

Let  $\check{c}_0 \in C^2(\overline{\Omega})$  satisfy

$$A_0 \frac{\partial \check{c}_0}{\partial n} > \|\mathbf{q}\|_{L^\infty(Q)} \check{c}_0(x) \quad \forall x \in S, \tag{2.20}$$

and

$$\|c^0\|_{L^\infty(\Omega)} < \check{c}_0(x) < \|c^0\|_{L^\infty(\Omega)} + 1 \quad \forall x \in \overline{\Omega}. \tag{2.21}$$

Let us define

$$\check{c}(t, x) := e^{\lambda t} \check{c}_0(x), \quad (t, x) \in Q, \tag{2.22}$$

for  $\lambda > 0$ . Then, for  $\lambda$  large enough, it is clear that

$$\theta \check{c}_t - \operatorname{div}(A \nabla \check{c} - \mathbf{q} \check{c}) + R + \theta_t \check{c} > 0 \quad \text{in } Q, \tag{2.23}$$

which means that

$$(\theta + \varphi'(\check{c})) \check{c}_t - \operatorname{div}(A \nabla \check{c} - \mathbf{q} \check{c}) + R + \theta_t \check{c} > 0 \quad \text{in } Q. \tag{2.24}$$

We have

$$\begin{cases} c_t = (\theta + \varphi'(c))^{-1} (\operatorname{div}(A \nabla c - \mathbf{q} c) - R) - \theta_t c & \text{in } Q, \\ A \nabla c \cdot \mathbf{n} = (\mathbf{q} \cdot \mathbf{n}) c - \alpha h(c) & \text{on } S_T, \end{cases} \tag{2.25}$$

and

$$\begin{cases} \check{c}_t > (\theta + \varphi'(\check{c}))^{-1} (\operatorname{div}(A \nabla \check{c} - \mathbf{q} \check{c}) - R) - \theta_t \check{c} & \text{in } Q, \\ A \nabla \check{c} \cdot \mathbf{n} > (\mathbf{q} \cdot \mathbf{n}) \check{c} - \alpha h(\check{c}) & \text{on } S_T. \end{cases} \tag{2.26}$$

Moreover,  $\check{c}(0, x) > c(0, x)$  in  $\overline{\Omega}$ .

Since we know that  $c > \delta e^{-KT} \min_{x \in \overline{\Omega}} \hat{c}_0(x)$  in  $Q$ , we can now apply Theorem 1 to  $c$  and  $\check{c}$  in  $Q$  to deduce that

$$c(t, x) < \check{c}(t, x), \quad (t, x) \in Q.$$

Thus, we can conclude that there exist  $c_{\min}, c_{\max}$  such that

$$0 < c_{\min} \leq c(t, x) \leq c_{\max}, \quad (t, x) \in Q. \tag{2.27}$$

### 3. Uniqueness of solutions in $C^{1,2}(\bar{Q})$

In this section, we prove the uniqueness of solutions of problem (1.1) in the space  $C^{1,2}(\bar{Q})$ .

Let  $c_1, c_2$  be two solutions of (1.1) belonging to  $C^{1,2}(\bar{Q})$ . From Sect. 2, we know that

$$0 < c_{\min} \leq c_1(t, x), c_2(t, x) \leq c_{\max}, \quad (t, x) \in Q. \tag{3.1}$$

Let us multiply the equation satisfied by  $c_1 - c_2$  by  $c_1 - c_2$ , integrate in  $\Omega$  and integrate by parts. This yields:

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \int_{\Omega} (\theta + \varphi'(c_1)) |c_1 - c_2|^2 dx - \frac{1}{2} \int_{\Omega} (-\theta_t + \varphi''(c_1)c_{1,t}) (c_1 - c_2)^2 dx \\ & + \int_{\Omega} (\varphi'(c_1) - \varphi'(c_2))(c_1 - c_2)c_{2,t} dx + \int_{\Omega} A |\nabla c_1 - \nabla c_2|^2 dx \\ & - \int_{\Omega} \mathbf{q} \cdot \nabla (c_1 - c_2)(c_1 - c_2) dx - \int_{\Gamma} A \frac{\partial}{\partial n} (c_1 - c_2)(c_1 - c_2) d\sigma \\ & + \int_{\Gamma} (\mathbf{q} \cdot \mathbf{n})(c_1 - c_2)^2 d\sigma = 0. \end{aligned} \tag{3.2}$$

We use that  $\theta_t \in L^\infty(\Omega \times (0, T))$  [see (2.5)],  $\varphi''(c_1) \in L^\infty(\Omega \times (0, T))$  [thanks to (2.3) and (3.1)] and  $\mathbf{q} \in L^\infty(\Omega \times (0, T))$ . We obtain:

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \int_{\Omega} (\theta + \varphi'(c_1)) |c_1 - c_2|^2 dx + \int_{\Omega} A |\nabla c_1 - \nabla c_2|^2 dx \\ & \leq K \left( \int_{\Omega} (1 + |c_{1,t}| + |c_{2,t}|) |c_1 - c_2|^2 + \int_{\Gamma_1} |c_1 - c_2|^2 d\sigma \right). \end{aligned} \tag{3.3}$$

Here, we have also used that  $|\alpha h(c_1) - \alpha h(c_2)| \leq K |c_1 - c_2|$  and the same property for  $\varphi'$ .

- We estimate the first term in the right-hand side:

$$\begin{aligned} \left| \int_{\Omega} |c_1 - c_2|^2 (|c_{1,t}| + |c_{2,t}|) dx \right| & \leq (\|c_{1,t}\|_{L^2(\Omega)} \\ & + \|c_{2,t}\|_{L^2(\Omega)}) \|c_1 - c_2\|_{L^4(\Omega)}^2. \end{aligned}$$

Using that

$$\|f\|_{L^4(\Omega)} \leq \|f\|_{L^2(\Omega)}^{1/4} \|f\|_{L^6(\Omega)}^{3/4},$$

we deduce that

$$\begin{aligned} & \left| \int_{\Omega} |c_1 - c_2|^2 (|c_{1,t}| + |c_{2,t}|) dx \right| \\ & \leq (\|c_{1,t}\|_{L^2(\Omega)} + \|c_{2,t}\|_{L^2(\Omega)}) \|c_1 - c_2\|_{L^2(\Omega)}^{1/2} \|c_1 - c_2\|_{L^6(\Omega)}^{3/2}. \end{aligned}$$

Using now Young’s inequality (for parameters 4 and 4/3), we obtain, for every  $\varepsilon \in [0, 1]$  there exists  $K_\varepsilon$  such that

$$\begin{aligned} & \left| \int_\Omega |c_1 - c_2|^2 (|c_{1,t}| + |c_{2,t}|) dx \right| \\ & \leq K_\varepsilon (\|c_{1,t}\|_{L^2(\Omega)}^4 + \|c_{2,t}\|_{L^2(\Omega)}^4) \|c_1 - c_2\|_{L^2(\Omega)}^2 + \varepsilon \|c_1 - c_2\|_{L^6(\Omega)}^2. \end{aligned}$$

From the continuous injection  $H^1(\Omega) \hookrightarrow L^6(\Omega)$  (recall that  $d = 2, 3$ ), we get

$$\begin{aligned} & \left| \int_\Omega |c_1 - c_2|^2 (1 + |c_{1,t}| + |c_{2,t}|) dx \right| \\ & \leq K'_\varepsilon (1 + \|c_{1,t}\|_{L^2(\Omega)}^4 + \|c_{2,t}\|_{L^2(\Omega)}^4) \|c_1 - c_2\|_{L^2(\Omega)}^2 + \varepsilon \|c_1 - c_2\|_{H^1(\Omega)}^2, \end{aligned} \tag{3.4}$$

where  $K'_\varepsilon$  does not depend on  $K_\varepsilon$ .

- For the second term in the right-hand side of (3.2), we consider a function  $\rho \in C^2(\overline{\Omega})$  satisfying  $\frac{\partial \rho}{\partial n} \geq 1$  on  $S$ . Then,

$$\begin{aligned} \int_\Gamma \frac{\partial \rho}{\partial n} |c_1 - c_2|^2 d\sigma &= 2 \int_\Omega (\nabla \rho \cdot \nabla (c_1 - c_2))(c_1 - c_2) dx \\ &+ \int_\Omega \Delta \rho (c_1 - c_2)^2 dx. \end{aligned}$$

From Young’s inequality, we easily deduce that for every  $\varepsilon \in [0, 1]$  there exists  $K_\varepsilon$  such that

$$\int_{\Gamma_1} |c_1 - c_2|^2 d\sigma \leq K_\varepsilon \|c_1 - c_2\|_{L^2(\Omega)}^2 + \varepsilon \|\nabla (c_1 - c_2)\|_{L^2(\Omega)}^2.$$

Putting this together with (3.4) and using (2.3), (2.4) and (2.5), we find

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \int_\Omega (\theta + \varphi'(c_1)) |c_1 - c_2|^2 dx + \int_\Omega A |\nabla c_1 - \nabla c_2|^2 dx \\ & \leq K_\varepsilon \theta_0^{-1} (1 + \|c_{1,t}\|_{L^2(\Omega)}^4 + \|c_{2,t}\|_{L^2(\Omega)}^4) \int_\Omega (\theta + \varphi'(c_1)) |c_1 - c_2|^2 dx \\ & + \varepsilon \int_\Omega A |\nabla c_1 - \nabla c_2|^2 dx. \end{aligned} \tag{3.5}$$

Finally, taking  $\varepsilon > 0$  small enough and using Gronwall’s Lemma, we deduce that  $c_1 = c_2$ .

#### 4. Existence and uniqueness of solutions in $C^{1+\beta/2, 2+\beta}(\overline{Q})$

Recall that  $\beta \in (0, 1)$  is fixed (2.9).

In order to apply an existence and uniqueness theorem, we need to define a new problem by truncating the function  $\varphi$ :



Let  $M_1, M_2$  be such that  $0 < M_1 < M_2$  and then let  $M := \begin{pmatrix} M_1 \\ M_2 \end{pmatrix}$ .

Then there exists  $\varphi_M \in C^3(\mathbb{R})$  such that

$$\begin{cases} \varphi_M(c) = \varphi(c) & \text{for } M_1 \leq c \leq M_2, \\ \varphi_M(c) = -\epsilon_M & \text{for } c \leq -\epsilon_M, \\ \varphi_M(c) = \varphi(M_2) + \epsilon_M & \text{for } c \geq M_2 + \epsilon_M, \\ \varphi'_M \geq 0, \end{cases}$$

for some  $\epsilon_M > 0$ .

Note, in particular, that  $\varphi'_M(c) = \varphi''_M(c) = \varphi'''_M(c) = 0$  for  $|c| > M_2 + \epsilon_M$  and that  $\varphi_M$  and its derivatives of up to order three are bounded.

Let us now define the new problem: find  $c_M$  such that

$$\begin{cases} \partial_t(\theta c_M + \varphi_M(c_M)) = \operatorname{div}(A \nabla c_M - \mathbf{q} c_M) - R & \text{in } Q, \\ \alpha h(c) = -(A \nabla c_M - \mathbf{q} c_M) \cdot \mathbf{n} & \text{on } I \times \Gamma_1, \\ 0 = (A \nabla c_M - \mathbf{q} c_M) \cdot \mathbf{n} & \text{on } I \times \Gamma_2, \\ c_M(0, x) = c^0(x) & \text{in } \Omega. \end{cases} \tag{4.1}$$

Let us make the following change of variables:

let  $y := \theta c_M + \varphi_M(c_M) - \theta(0, x)c^0(x) - \varphi_M(c^0)$ .

Note that  $y$  is strictly monotonically increasing in the variable  $c_M$  (recall that  $\theta \geq \theta_0 > 0$  in  $\overline{Q}$  and  $\varphi'_M \geq 0$ ). Thus, we have  $c_M = k(t, x, y)$  with  $k$  strictly monotonically increasing in the variable  $y$ .

Moreover,  $k$  is three times continuously differentiable with respect to  $y$ .

We can write the problem as follows:

$$\begin{cases} \partial_t y - \operatorname{div}(A \nabla k - \mathbf{q} k) + R = 0 & \text{in } Q, \\ (A \nabla k - \mathbf{q} k) \cdot \mathbf{n} + \alpha h(k) = 0 & \text{on } I \times \Gamma_1, \\ (A \nabla k - \mathbf{q} k) \cdot \mathbf{n} = 0 & \text{on } I \times \Gamma_2, \\ y(0, x) = 0 & \text{in } \Omega. \end{cases} \tag{4.2}$$

We use the following notations for derivatives:

$$\frac{d}{dx}[a(x, u(x))] = \frac{\partial a}{\partial x} + \frac{\partial a}{\partial u} u_x = a_x + a_u u_x.$$

The equation in  $Q$  gives:

$$\partial_t y - \sum_i \frac{d}{dx_i} \left( A \frac{d}{dx_i} k \right) + \sum_i \frac{d}{dx_i} (q_i k) + R = 0.$$

Using the chain rule yields:

$$\partial_t y - \sum_i A \frac{d^2}{dx_i^2} k - \sum_i \frac{d}{dx_i} A \frac{d}{dx_i} k + \sum_i \left( k \frac{d}{dx_i} q_i + q_i \frac{d}{dx_i} k \right) + R = 0.$$

We obtain:

$$\begin{aligned} \partial_t y - A \sum_i & \left[ k_{x_i x_i} + k_y y_{x_i x_i} + k_{y x_i} y_{x_i} + k_{x_i y} y_{x_i} + k_{y y} y_{x_i}^2 \right] \\ & - \sum_i \left[ A_{x_i} k_{x_i} + A_{x_i} k_y y_{x_i} - k q_{i x_i} - q_i k_{x_i} - q_i k_y y_{x_i} \right] + R = 0. \end{aligned}$$

The equation in  $I \times \partial(\Omega)$  gives:

$$\sum_i \left( A \frac{d}{dx_i} k - q_i k \right) \cos(\mathbf{n}, x_i) + \alpha h(k) = 0.$$

Using the chain rule again yields:

$$A \sum_i k_y y_{x_i} \cos(\mathbf{n}, x_i) + \sum_i (A k_{x_i} - q_i k) \cos(\mathbf{n}, x_i) + \alpha h(k) = 0.$$

Finally, we can see that our problem is of the general form

$$\begin{cases} Ly := y_t - a_{ij}(x, t, y) y_{x_i x_j} + b(x, t, y, y_x) = 0, \\ L^{(S)} y := a_{ij}(x, t, y) y_{x_j} \cos(\mathbf{n}, x_i) + \psi(x, t, y)|_{S_T} = 0, \\ y|_{t=0} = 0, \end{cases} \tag{4.3}$$

with

$$\begin{cases} a_{ij} = 0 \text{ for } i \neq j, \\ a_{ii} = A k_y, \\ b = -A \sum_i \left[ k_{x_i x_i} + k_{y x_i} y_{x_i} + k_{x_i y} y_{x_i} + k_{y y} y_{x_i}^2 \right] \\ \quad - \sum_i \left[ A_{x_i} k_{x_i} + A_{x_i} k_y y_{x_i} - k q_{i x_i} - q_i k_{x_i} - q_i k_y y_{x_i} \right] + R, \\ \psi = \sum_i (A k_{x_i} - q_i k) \cos(\mathbf{n}, x_i) + \alpha h(k). \end{cases} \tag{4.4}$$

We can now apply the following theorem to problem (4.3):

**THEOREM 2.** ([7, Theorem 7.4 p. 491]) *Suppose the following conditions are fulfilled:*

*There exists  $\mu_1 > 0$  and  $c_0, c_1, c_2, c_3, c_4 \geq 0$  such that for arbitrary  $y$ ,*

$$0 \leq \sum_{i,j} a_{ij}(x, t, y) \xi_i \xi_j \leq \mu_1 \xi^2 \quad \text{for } (t, x) \in \bar{Q}, \tag{4.5a}$$

$$-y b(x, t, y, p) \leq c_0 p^2 + c_1 y^2 + c_2 \quad \text{for } (t, x) \in \bar{Q}, \tag{4.5b}$$

$$-y \psi(x, t, y) \leq c_3 y^2 + c_4 \quad \text{for } (t, x) \in S_T, \tag{4.5c}$$

$$\sum_{i,j} a_{ij}(x, t, y) \xi_i \xi_j \geq \nu_1 \xi^2 \quad \text{for } (t, x) \in S_T. \tag{4.5d}$$

*There exists  $\nu, \mu > 0$  such that for  $(t, x) \in \bar{Q}$ ,  $|y| \leq N$  and for arbitrary  $p$  the functions  $a_{ij}(x, t, y)$ ,  $b(x, t, y, p)$  and  $\psi(x, t, y)$  are continuous in their arguments, possess the derivatives entering into the following conditions and satisfy these*

conditions:

$$v\xi^2 \leq \sum_{i,j} a_{ij}(x, t, y)\xi_i\xi_j \leq \mu\xi^2, \tag{4.6a}$$

$$\left| \frac{\partial a_{ij}(x, t, y)}{\partial y}, \frac{\partial a_{ij}}{\partial x}, \psi, \frac{\partial \psi}{\partial y}, \frac{\partial \psi}{\partial x} \right| \leq \mu, \tag{4.6b}$$

$$|b(x, t, y, p)| \leq \mu(1 + p^2), \tag{4.6c}$$

$$|\psi_{yy}(x, t, y), \psi_{yx}, \psi_{yt}, a_{ij_t}, \psi_t| \leq \mu, \tag{4.7a}$$

$$|b_p|(1 + |p|) + |b_y| + |b_t| \leq \mu(1 + p^2), \tag{4.7b}$$

$$|a_{ij_{yy}}, a_{ij_{yt}}, a_{ij_{yx_j}}, a_{ij_{x_jt}}| \leq \mu. \tag{4.7c}$$

For  $(t, x) \in \overline{Q}$ ,  $|y| \leq N$  and  $|p| \leq N$ , the functions  $a_{ij_x}(x, t, y)$  are Hölder continuous in the variables  $x$  with exponent  $\beta$ ,  $\psi_x(x, t, y)$  is Hölder continuous in  $x$  and  $t$  with exponent  $\beta$  and  $\beta/2$ , respectively, and  $b(x, t, y, p)$  is Hölder continuous in  $x$  with exponent  $\beta$ . (4.8)

$$S \in C^{2+\beta}. \tag{4.9a}$$

$$\psi(x, 0, 0)|_{x \in S} = 0. \tag{4.9b}$$

Then problem (4.3) has a unique solution  $y(t, x)$  in the class  $C^{1+\beta/2, 2+\beta}(\overline{Q})$ .

Let us verify hypotheses (4.5a) to (4.9b) for our problem:

**Proof of (4.5a) (4.5d) (4.6a).** We have

$$k_y = \frac{1}{y_k \circ k} = \frac{1}{\theta + \varphi'_M(k)},$$

and since  $0 < A_0 \leq A(t, x) \leq A_m$  in  $\overline{Q}$  and  $0 < \theta_0 \leq \theta(t, x) + \varphi'_M(k) < +\infty$  in  $\overline{Q} \times \mathbb{R}$ , it follows that (4.5a), (4.5d) and (4.6a) hold.

**Proof of (4.5b) (4.5c).** We have

$$\begin{aligned} -yb(x, t, y, p) &= \sum_i \left[ Ak_{x_i x_i} y + A_{x_i} k_{x_i} y - kq_{i x_i} y - q_i k_{x_i} y \right] - Ry \\ &+ A \sum_i \left[ k_{y x_i} p_i y + k_{x_i y} p_i y + k_{yy} p_i^2 y \right] \\ &+ \sum_i \left[ A_{x_i} k_y p_i y - q_i k_y p_i y \right]. \end{aligned}$$

– Terms not involving  $p$ , for example  $Ak_{x_i x_i} y$ , are handled in this way:

$$\begin{aligned} k_{x_i x_j} &= -\frac{\theta_{x_i x_j} k}{\theta + \varphi'_M(k)} + \frac{2\theta_{x_i} \theta_{x_j} k}{(\theta + \varphi'_M(k))^2} - \frac{\theta_{x_i} \theta_{x_j} \varphi''_M(k) k^2}{(\theta + \varphi'_M(k))^3} \\ &+ \frac{\theta^0_{x_i x_j} c^0 + \theta^0_{x_i} c^0_{x_j} + (\theta^0 + \varphi'_M(c^0)) c^0_{x_i x_j} + (\theta^0_{x_j} + \varphi''_M(c^0) c^0_{x_j}) c^0_{x_i}}{\theta + \varphi'_M(k)} \end{aligned}$$

$$\begin{aligned}
 & - \left( \theta_{x_i}^0 c^0 + (\theta^0 + \varphi'_M(c^0))c_{x_i}^0 \right) \\
 & \times \left( \frac{\theta_{x_j}}{(\theta + \varphi'_M(k))^2} + \frac{\varphi''_M(k)(\theta_{x_i}^0 c^0 + (\theta^0 + \varphi'_M(c^0))c_{x_i}^0)}{(\theta + \varphi'_M(k))^3} - \frac{\varphi''_M(k)\theta_{x_i} k}{(\theta + \varphi'_M(k))^3} \right).
 \end{aligned}$$

We have  $\theta_0 \leq \theta(t, x) + \varphi'_M(k) < +\infty$ . Moreover, for  $|y|$  large enough there holds  $k = \theta^{-1}y + c_t$  (with  $c_t$  bounded and independent of  $y$ ) and  $\varphi''_M(k) = 0$ .

Taking into account that  $\theta, A, \theta^0, c^0$  and their space derivatives of up to order two are bounded, it follows that there exists  $c_{3a}, c_{3b} \geq 0$  such that for arbitrary  $y$

$$|Ak_{x_i x_i} y| \leq c_{3a} y^2 + c_{3b} \quad \text{for } (t, x) \in \overline{Q}.$$

Remaining terms not involving  $p$  are handled similarly.

- $k_y, k_{yx_i}$  and  $k_{x_i y}$ , the derivatives appearing in terms involving  $p$ , can be bounded independently of  $y$ . In the case of the term  $Ak_{yx_i} p_i y$ , we have

$$k_{yx_i} = \frac{-\theta_{x_i}}{(\theta + \varphi'_M(k))^2} + \frac{\theta_{x_i} \varphi''_M(k) k}{(\theta + \varphi'_M(k))^3} - \frac{\varphi''_M(k) (\theta_{x_i}^0 c^0 + (\theta^0 + \varphi'_M(c^0))c_{x_i}^0)}{(\theta + \varphi'_M(k))^3},$$

which leads to the fact that there exists  $c_{t_2}, c_{5a}, c_{5b} \geq 0$  such that for arbitrary  $y$

$$|Ak_{yx_i} p_i y| \leq c_{t_2} |p_i| |y| \leq c_{5a} p^2 + c_{5b} y^2 \quad \text{for } (t, x) \in \overline{Q}.$$

- The term  $Ak_{yy} p_i^2 y$  remains. We have

$$k_{yy} = \frac{-\varphi''_M(k) k_y}{(\theta + \varphi'_M(k))^2} = \frac{-\varphi''_M(k)}{(\theta + \varphi'_M(k))^3},$$

which vanishes for  $|y|$  large enough. It follows that there exists  $c_6 \geq 0$  such that for arbitrary  $y$

$$|Ak_{yy} p_i^2 y| \leq c_6 p^2 \quad \text{for } (t, x) \in \overline{Q}.$$

Consequently, (4.5b) holds.

(4.5c) can be verified in the same way as (4.5b).

**Proof of (4.6b) (4.6c) (4.7a) (4.7b) (4.7c).** It is easy to see that under the assumptions we made, all appearing quantities in these hypotheses are defined and bounded, and thus, it is clear that these conditions are verified.

**Proof of (4.8).** We have

$$\begin{aligned}
 \frac{\partial a_{ii}(x, t, y)}{\partial x_j} &= A_{x_j} k_y + Ak_{yx_j}, \\
 \frac{\partial \psi}{\partial x_j} &= \sum_i [(A_{x_j} k_{x_i} + Ak_{x_i x_j} - q_{i, x_j} k - q_i k_{x_j}) n_i + (Ak_{x_i} - q_i k) n_{i, x_j}] \\
 &\quad + \alpha h'(k) k_{x_j} + \alpha_{x_j} h(k),
 \end{aligned}$$

and one can easily verify that under the assumptions we made, the Hölder continuity hypotheses on  $a_{ijx}(x, t, y), \psi_x(x, t, y)$  and  $b(x, t, y, p)$  required by (4.8) hold true.

**Proof of (4.9a).** We made the assumption that  $S \in C^{2+\beta}$ .

**Proof of (4.9b).** We have the following initial and boundary compatibility condition:

$$(A\nabla c^0 - \mathbf{q}c^0) \cdot \mathbf{n} + \alpha h(c^0) = 0 \quad \text{on } S,$$

which, since  $k|_{t=0} = c^0$ , leads to

$$\psi(x, 0, 0) = \sum_i (Ac_{x_i}^0 - q_i c^0) \cos(\mathbf{n}, x_i) + \alpha h(c^0) = 0 \quad \text{on } S,$$

and (4.9b) holds.

Thus, problem (4.3) has a unique solution  $y$  in the class  $C^{1+\beta/2, 2+\beta}(\overline{Q})$ .

Consequently, problem (4.1) has a unique solution  $c_M$  in the class  $C^{1+\beta/2, 2+\beta}(\overline{Q})$ .

Now, note that we can find estimates for solutions  $c_M$  of problem (4.1) in exactly the same way we did for problem (1.1) in Sect. 2. Moreover, one can easily see that

$c_M$  can be bounded independently of  $M : \forall M = \begin{pmatrix} M_1 \\ M_2 \end{pmatrix}, 0 < M_1 < M_2,$

$$0 < c_{\min} \leq c_M(t, x) \leq c_{\max}, \quad (t, x) \in Q. \tag{4.10}$$

We can then choose  $M$  so that  $M_1 < c_{\min}$  and  $M_2 > c_{\max}$ . It follows that the unique solution  $c_M$  of problem (4.1) is also a solution of the original problem (1.1). Thus, using the fact that problem (1.1) has at most one solution in the space  $C^{1,2}(\overline{Q})$  which was proven in Sect. 3, we can deduce that problem (1.1) has a unique solution in the space  $C^{1+\beta/2, 2+\beta}(\overline{Q})$ .

### 5. Shape optimization

In this section, we use the tools of shape optimization presented in [4, 11] and [6] to find root shapes that increase the amount of absorbed P. More specifically, we want to deform  $\Omega$  so as to maximize the shape functional

$$J(c) = \int_0^T \int_{\Gamma_1} \alpha h(c), \tag{5.1}$$

where  $|\Omega| = a$  given constant.

We also assume that  $A$  and  $\mathbf{q}$  are constants and we take  $R = 0$ .

We introduce a vector field  $\mathbf{V} \in C^2(\mathbb{R}^d, \mathbb{R}^d)$  and we consider  $\Omega_s = (Id + s\mathbf{V})(\Omega)$  where  $s$  is a small parameter.

Let  $c_s$  be the unique solution of the problem on the perturbed domain:

$$\begin{cases} \partial_t(\theta c_s + \varphi(c_s)) = \operatorname{div}(A\nabla c_s - \mathbf{q}c_s) & \text{in } I \times \Omega_s, \\ \alpha h(c_s) = - (A\nabla c_s - \mathbf{q}c_s) \cdot \mathbf{n} & \text{on } I \times \Gamma_{1,s}, \\ 0 = - (A\nabla c_s - \mathbf{q}c_s) \cdot \mathbf{n} & \text{on } I \times \Gamma_{2,s}, \\ c_s(0, x) = c^0 (Id + s\mathbf{V})^{-1}(x) & \text{in } \Omega_s. \end{cases} \tag{5.2}$$

Let us now denote by  $c'$  the derivative of  $c$  with respect to the domain:  $c' = \frac{d}{ds}c_s|_{s=0}$ . According to [6, Prop. 5.4.18 p. 201], the derivative of the functional  $J$  at  $\Omega$  in the direction  $\mathbf{V}$  is given by

$$dJ(c, \mathbf{V}) = \int_0^T \left( \int_{\Gamma_1} \alpha h'(c)c' + \int_{\Gamma_1} \alpha Hh(c)(\mathbf{V} \cdot \mathbf{n}) + \int_{\Gamma_1} \frac{\partial(\alpha h(c))}{\partial n}(\mathbf{V} \cdot \mathbf{n}) \right) \tag{5.3}$$

where  $H$  is the mean curvature of  $\Gamma$ .

We first need to find the equation satisfied by  $c'$ :

The solution  $c$  of the initial problem satisfies

$$\int_0^T \int_{\Omega} \partial_t(\theta c + \varphi(c))v + \int_0^T \int_{\Omega} A \nabla c \cdot \nabla v - \int_0^T \int_{\Omega} c \mathbf{q} \cdot \nabla v + \int_0^T \int_{\Gamma_1} \alpha h(c)v = 0 \tag{5.4}$$

for all  $v \in H^1(\Omega)$  such that  $v(T, \cdot) = 0$ .

Differentiating (5.4) using rules presented in [6] gives

$$\begin{aligned} & \int_0^T \int_{\Omega} \partial_t(\theta c' + \varphi'(c)c')v + \int_0^T \int_{\Gamma} \partial_t(\theta c + \varphi(c))v(\mathbf{V} \cdot \mathbf{n}) \\ & + \int_0^T \int_{\Omega} A \nabla c' \cdot \nabla v + \int_0^T \int_{\Gamma} A \nabla c \cdot \nabla v(\mathbf{V} \cdot \mathbf{n}) \\ & - \int_0^T \int_{\Omega} c' \mathbf{q} \cdot \nabla v - \int_0^T \int_{\Gamma} c \mathbf{q} \cdot \nabla v(\mathbf{V} \cdot \mathbf{n}) + \int_0^T \int_{\Gamma_1} \alpha h'(c)c'v \\ & + \int_0^T \int_{\Gamma_1} H \alpha h(c)v(\mathbf{V} \cdot \mathbf{n}) + \int_0^T \int_{\Gamma_1} \frac{\partial(\alpha h(c)v)}{\partial n}(\mathbf{V} \cdot \mathbf{n}) = 0. \end{aligned} \tag{5.5}$$

First taking  $v$  in  $\mathcal{D}(\Omega)$ , we obtain that

$$\frac{\partial}{\partial t} (\theta c' + \varphi'(c)c') - A \Delta c' + \mathbf{q} \cdot \nabla c' = 0 \text{ in } \mathcal{Q}. \tag{5.6}$$

Integrating by parts  $\int_{\Omega} (A \nabla c' - c' \mathbf{q}) \cdot \nabla v$  in (5.5) and using (5.6) gives

$$\begin{aligned} & - \int_0^T \int_{\Gamma} A \frac{\partial c'}{\partial n} v - c' v \mathbf{q} \cdot \mathbf{n} = \int_0^T \int_{\Gamma} \partial_t(\theta c + \varphi(c))v(\mathbf{V} \cdot \mathbf{n}) \\ & + \int_0^T \int_{\Gamma} A \nabla c \cdot \nabla v(\mathbf{V} \cdot \mathbf{n}) - \int_0^T \int_{\Gamma} c \mathbf{q} \cdot \nabla v(\mathbf{V} \cdot \mathbf{n}) \\ & + \int_0^T \int_{\Gamma_1} \alpha h'(c)c'v + \int_0^T \int_{\Gamma_1} H \alpha h(c)v(\mathbf{V} \cdot \mathbf{n}) + \int_0^T \int_{\Gamma_1} \frac{\partial(\alpha h(c)v)}{\partial n}(\mathbf{V} \cdot \mathbf{n}). \end{aligned} \tag{5.7}$$

We have

$$\int_0^T \int_{\Gamma} A \nabla c \cdot \nabla v(\mathbf{V} \cdot \mathbf{n}) = \int_0^T \int_{\Gamma} \left( A \nabla_T c \cdot \nabla_T v + A \frac{\partial c}{\partial n} \frac{\partial v}{\partial n} \right) (\mathbf{V} \cdot \mathbf{n}), \tag{5.8}$$

where  $\nabla_T$  is the tangential part of the gradient.

An integration by parts gives:

$$\int_{\Gamma} (A \nabla_T c \cdot \nabla_T v)(\mathbf{V} \cdot \mathbf{n}) = - \int_{\Gamma} A \nabla_T c \cdot \nabla_T (\mathbf{V} \cdot \mathbf{n}) v - \int_{\Gamma} A \Delta_T c (\mathbf{V} \cdot \mathbf{n}) v, \tag{5.9}$$

where  $\Delta_T c = \operatorname{div}_T(\nabla_T c)$  is the Laplace-Beltrami operator.

Now, using [6, Prop. 5.4.12 p. 196], we have

$$\begin{aligned} A \Delta_T c &= A \Delta c - AH \frac{\partial c}{\partial n} - A \frac{\partial^2 c}{\partial n^2} \\ &= \partial_t(\theta c + \varphi(c)) + \operatorname{div}(\mathbf{q}c) - AH \frac{\partial c}{\partial n} - A \frac{\partial^2 c}{\partial n^2}. \end{aligned} \tag{5.10}$$

Then (5.7) reads

$$\begin{aligned} & - \int_0^T \int_{\Gamma} A \frac{\partial c'}{\partial n} v - c' v \mathbf{q} \cdot \mathbf{n} = - \int_0^T \int_{\Gamma} A \nabla_T c \cdot \nabla_T (\mathbf{V} \cdot \mathbf{n}) v \\ & - \int_0^T \int_{\Gamma} \left( \operatorname{div}(\mathbf{q}c) - AH \frac{\partial c}{\partial n} - A \frac{\partial^2 c}{\partial n^2} \right) (\mathbf{V} \cdot \mathbf{n}) v \\ & + \int_0^T \int_{\Gamma} A \frac{\partial c}{\partial n} \frac{\partial v}{\partial n} (\mathbf{V} \cdot \mathbf{n}) - \int_0^T \int_{\Gamma} c \mathbf{q} \cdot \nabla_T v (\mathbf{V} \cdot \mathbf{n}) - \int_0^T \int_{\Gamma} c \mathbf{q} \cdot \mathbf{n} \frac{\partial v}{\partial n} (\mathbf{V} \cdot \mathbf{n}) \\ & + \int_0^T \int_{\Gamma_1} \alpha h'(c) c' v + \int_0^T \int_{\Gamma_1} H \alpha h(c) v (\mathbf{V} \cdot \mathbf{n}) + \int_0^T \int_{\Gamma_1} \frac{\partial(\alpha h(c) v)}{\partial n} (\mathbf{V} \cdot \mathbf{n}). \end{aligned} \tag{5.11}$$

Moreover, since

$$\begin{aligned} - \int_{\Gamma} c \mathbf{q} \cdot \nabla_T v (\mathbf{V} \cdot \mathbf{n}) &= - \int_{\Gamma} \operatorname{div}_T(\mathbf{q}c (\mathbf{V} \cdot \mathbf{n}) v) + \int_{\Gamma} \operatorname{div}_T(\mathbf{q}c (\mathbf{V} \cdot \mathbf{n})) v \\ &= - \int_{\Gamma} H \mathbf{q} \cdot \mathbf{n} c (\mathbf{V} \cdot \mathbf{n}) v + \int_{\Gamma} \operatorname{div}_T(\mathbf{q}c (\mathbf{V} \cdot \mathbf{n})) v, \end{aligned} \tag{5.12}$$

we can see by using the boundary conditions verified by  $c$  that

$$\int_0^T \int_{\Gamma} (\mathbf{V} \cdot \mathbf{n}) \left( H v + \frac{\partial v}{\partial n} \right) \left( A \frac{\partial c}{\partial n} - c \mathbf{q} \cdot \mathbf{n} \right) + \int_0^T \int_{\Gamma_1} (\mathbf{V} \cdot \mathbf{n}) \left( H v + \frac{\partial v}{\partial n} \right) \alpha h(c) = 0. \tag{5.13}$$

After using this simplification, (5.11) reads

$$\begin{aligned}
 & - \int_0^T \int_{\Gamma} A \frac{\partial c'}{\partial n} v - c' v \mathbf{q} \cdot \mathbf{n} = - \int_0^T \int_{\Gamma} A \nabla_T c \cdot \nabla_T (\mathbf{V} \cdot \mathbf{n}) v \\
 & - \int_0^T \int_{\Gamma} \left( \operatorname{div}(\mathbf{q}c) - A \frac{\partial^2 c}{\partial n^2} \right) (\mathbf{V} \cdot \mathbf{n}) v \\
 & + \int_{\Gamma} \operatorname{div}_T(\mathbf{q}c(\mathbf{V} \cdot \mathbf{n})) v + \int_0^T \int_{\Gamma_1} \alpha h'(c) c' v \\
 & + \int_0^T \int_{\Gamma_1} \frac{\partial(\alpha h(c))}{\partial n} v (\mathbf{V} \cdot \mathbf{n}), \tag{5.14}
 \end{aligned}$$

from which we can deduce the boundary conditions for  $c'$ .

Finally, the equation satisfied by  $c'$  is

$$\frac{\partial}{\partial t} (\theta c' + \varphi'(c) c') - A \Delta c' + \mathbf{q} \cdot \nabla c' = 0 \quad \text{in } Q, \tag{5.15}$$

with boundary conditions

$$\begin{cases}
 A \frac{\partial c'}{\partial n} - c' \mathbf{q} \cdot \mathbf{n} + \alpha h'(c) c' = \left( -A \frac{\partial^2 c}{\partial n^2} - \frac{\partial(\alpha h(c))}{\partial n} + \mathbf{q} \cdot \nabla c \right) (\mathbf{V} \cdot \mathbf{n}) \\
 \quad + A \nabla_T (\mathbf{V} \cdot \mathbf{n}) \cdot \nabla_T c - \nabla_T (c \mathbf{V} \cdot \mathbf{n}) \cdot \mathbf{q} \quad \text{on } I \times \Gamma_1, \\
 A \frac{\partial c'}{\partial n} - c' \mathbf{q} \cdot \mathbf{n} = \left( -A \frac{\partial^2 c}{\partial n^2} + \mathbf{q} \cdot \nabla c \right) (\mathbf{V} \cdot \mathbf{n}) \\
 \quad + A \nabla_T (\mathbf{V} \cdot \mathbf{n}) \cdot \nabla_T c - \nabla_T (c \mathbf{V} \cdot \mathbf{n}) \cdot \mathbf{q} \quad \text{on } I \times \Gamma_2,
 \end{cases} \tag{5.16}$$

and initial value

$$c'(0, x) = 0. \tag{5.17}$$

In order to get rid of the shape derivative  $c'$  (which we would have to compute for every choice of  $\mathbf{V}$ ) in the expression of  $dJ$  (5.3), we use the adjoint state technique. Let us introduce  $p$  the solution to the following adjoint state problem:

$$\begin{cases}
 -(\theta + \varphi'(c)) \partial_t p - \operatorname{div}(A \nabla p) - \mathbf{q} \cdot \nabla p = 0 \quad \text{in } Q, \\
 (A \nabla p) \cdot \mathbf{n} + \alpha h'(c) p = \alpha h'(c) \quad \text{on } I \times \Gamma_1, \\
 (A \nabla p) \cdot \mathbf{n} = 0 \quad \text{on } I \times \Gamma_2, \\
 p(T, x) = 0 \quad \text{in } \Omega.
 \end{cases} \tag{5.18}$$

See for example [3, Theorem 2 p. 144] for existence of a solution to this problem.

The only integral we need to get rid of in (5.3) is

$$\mathcal{I} := \int_0^T \int_{\Gamma_1} \alpha h'(c) c'. \tag{5.19}$$

Using the boundary conditions satisfied by  $p$ , we have

$$\mathcal{I} = \int_0^T \int_{\Gamma_1} \alpha h'(c) c' p + \int_0^T \int_{\Gamma} c' (A \nabla p) \cdot \mathbf{n}. \tag{5.20}$$



Integrations by parts give

$$\mathcal{I} = \int_0^T \int_{\Gamma_1} \alpha h'(c) c' p + \int_0^T \int_{\Omega} c' A \Delta p - p A \Delta c' + \int_0^T \int_{\Gamma} A p \nabla c' \cdot \mathbf{n}. \tag{5.21}$$

From the equations in  $c'$  and  $p$ , we have

$$\partial_t [c' p(\theta + \varphi'(c))] + c' A \Delta p - p A \Delta c' + \mathbf{q} \cdot \nabla(c' p) = 0, \tag{5.22}$$

which after integration gives

$$\int_0^T \int_{\Omega} c' A \Delta p - p A \Delta c' = - \int_0^T \int_{\Gamma} c' p \mathbf{q} \cdot \mathbf{n}. \tag{5.23}$$

We deduce

$$\mathcal{I} = \int_0^T \int_{\Gamma_1} \alpha h'(c) c' p + \int_0^T \int_{\Gamma} A p \nabla c' \cdot \mathbf{n} - c' p \mathbf{q} \cdot \mathbf{n}. \tag{5.24}$$

Using the boundary conditions satisfied by  $c'$  given by (5.16), we obtain

$$\begin{aligned} \mathcal{I} = & \int_0^T \int_{\Gamma} p \left( \left( -A \frac{\partial^2 c}{\partial n^2} + \mathbf{q} \cdot \nabla c \right) (\mathbf{V} \cdot \mathbf{n}) + A \nabla_T (\mathbf{V} \cdot \mathbf{n}) \cdot \nabla_T c - \nabla_T (c \mathbf{V} \cdot \mathbf{n}) \cdot \mathbf{q} \right) \\ & - \int_0^T \int_{\Gamma_1} p \frac{\partial(\alpha h(c))}{\partial n} (\mathbf{V} \cdot \mathbf{n}). \end{aligned} \tag{5.25}$$

Integrations by parts lead to

$$\begin{aligned} \mathcal{I} = & \int_0^T \int_{\Gamma} \left( p \left( -A \frac{\partial^2 c}{\partial n^2} + \mathbf{q} \cdot \nabla c \right) - \operatorname{div}_T (p A \nabla_T c) + c \operatorname{div}_T (p \mathbf{q}) \right) (\mathbf{V} \cdot \mathbf{n}) \\ & - \int_0^T \int_{\Gamma_1} p \frac{\partial(\alpha h(c))}{\partial n} (\mathbf{V} \cdot \mathbf{n}). \end{aligned} \tag{5.26}$$

Note that the shape gradient  $dJ$  is now expressed in the following convenient way:

$$dJ(c, \mathbf{V}) = \int_{\Gamma} j(\mathbf{V} \cdot \mathbf{n}),$$

where  $j$  does not depend on  $\mathbf{V}$ .

With that in mind, a simple yet effective approach to maximize  $J$  consists in choosing  $\mathbf{V}$  such that  $\mathbf{V} \cdot \mathbf{n} = j$ , i.e.,  $\mathbf{V} = j\mathbf{n}$ . This brings

$$J(c, \mathbf{V}) = \int_{\Gamma} j^2 > 0,$$

which ensures that  $J$  increases as the domain is iteratively deformed.

Note that this method restricts the choice of the deformation, as  $\mathbf{V}$  is taken colinear with  $\mathbf{n}$ .

From a numerical point of view, we still need to transform the expression of  $j$  in order to avoid numerical computations of second-order derivatives. We have

$$-\operatorname{div}_T(pA\nabla_T c) = -A\nabla p\nabla_T c - pA\Delta_T c. \quad (5.27)$$

Using [6, Prop. 5.4.12 p. 196] again as in (5.10) yields

$$-\operatorname{div}_T(pA\nabla_T c) = -A\nabla p\nabla_T c - p \left( \partial_t(\theta c + \varphi(c)) + \operatorname{div}(\mathbf{q}c) - AH \frac{\partial c}{\partial n} - A \frac{\partial^2 c}{\partial n^2} \right). \quad (5.28)$$

Finally, using (5.28) in (5.26), we can express  $dJ(c, \mathbf{V})$  as

$$\begin{aligned} dJ(c, \mathbf{V}) &= \mathcal{I} + \int_0^T \left( \int_{\Gamma_1} \alpha Hh(c)(\mathbf{V} \cdot \mathbf{n}) + \int_{\Gamma_1} \frac{\partial(\alpha h(c))}{\partial n} (\mathbf{V} \cdot \mathbf{n}) \right) \\ &= \int_0^T \int_{\Gamma} \left( -A\nabla p\nabla_T c - (\partial_t(\theta c + \varphi(c))p + pAH \frac{\partial c}{\partial n} + c\nabla_T p \cdot \mathbf{q}) (\mathbf{V} \cdot \mathbf{n}) \right. \\ &\quad \left. + \int_0^T \int_{\Gamma_1} \left( -p \frac{\partial(\alpha h(c))}{\partial n} + \alpha Hh(c) + \frac{\partial(\alpha h(c))}{\partial n} \right) (\mathbf{V} \cdot \mathbf{n}). \right. \end{aligned} \quad (5.29)$$

Numerical resolution of the state and adjoint equations in two spatial dimensions is carried out using the free finite element software FreeFEM++ [5]. Spatial discretization is done using Lagrange P2 finite elements.

The backward Euler method is applied for the discretization in time. Nonlinearities in the state equation are handled by Newton's method. A built-in adaptive anisotropic mesh refinement algorithm is used in order to improve accuracy near the boundary while preserving an acceptable computational cost.

The constant volume constraint is enforced by a Lagrange multiplier. Additionally, a minimum diameter constraint is put on the shape in order to prevent unsuitable deformations of the domain.

Numerical values used in the example illustrated in Figs. 2, 3, 4 are as follows:

- $F_m = 0.282 \mu\text{mol cm}^{-2} \text{d}^{-1}$ ,  $K_m = 5.8 \times 10^{-3} \mu\text{mol cm}^{-3}$ ,  $c^0 = 2.9 \times 10^{-3} \mu\text{mol cm}^{-3}$ ,
- $\kappa = 6.15$ ,  $b = 0.72$ ,
- $\theta = 0.35 \text{ cm}^3 \text{ cm}^{-3}$ ,
- $A = 0.102 \text{ cm}^2 \text{d}^{-1}$ ,
- $\mathbf{q} = 0$ ,  $R = 0$ .
- The initial shape is an ellipse of diameters 1.33 and 2.66 cm.

In order to make sure that the boundary is not deformed in the region of the root collar where  $0 \leq \alpha < 1$  as well as to enforce the minimum diameter constraint, the deformation field  $\mathbf{V} = j\mathbf{n}$  is locally modified so as to vanish where the perturbed shape breaks these constraints. This is achieved by multiplying  $\mathbf{V}$  by  $C^\infty(\mathbb{R}^d)$  cutoff functions taking values in  $[0, 1]$  whose supports do not intersect the critical regions. This puts more and more restrictions on  $\mathbf{V}$  as the shape evolves from the initial elliptic shape and causes the decrease in the shape gradient from iteration 200 to iteration 500 as we can see in Fig. 4. After iteration 500, the diameter constraint inhibits the

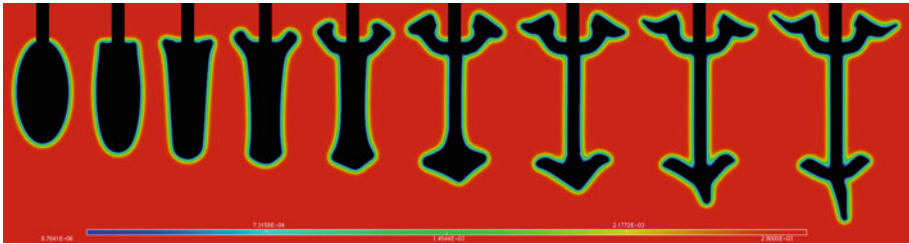


Figure 2. Snapshots of the domain and P concentration at different steps of the shape optimization process

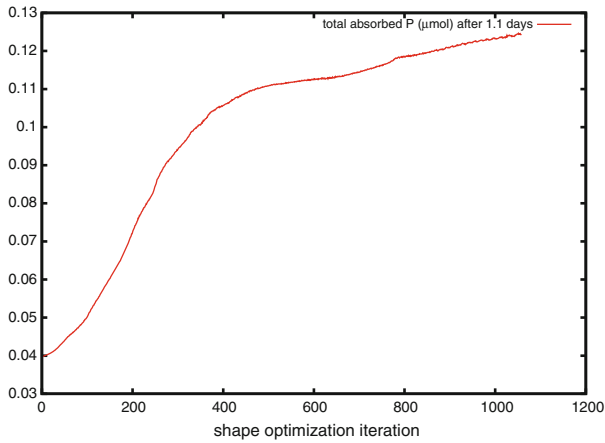


Figure 3. Evolution of the total amount of absorbed P during the optimization process

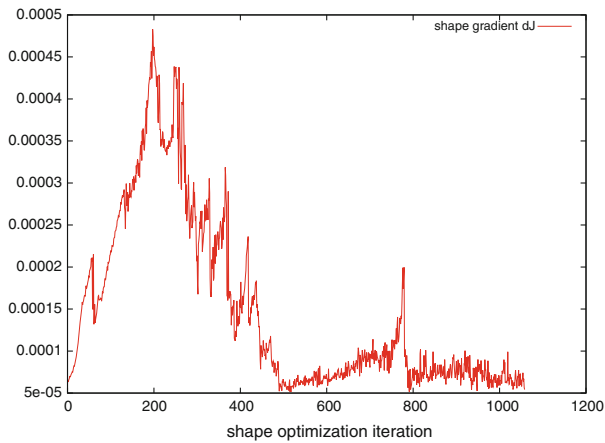


Figure 4. Evolution of the shape gradient  $dJ$  during the optimization process

optimization process. We observe residual oscillations of the shape gradient, and the computed shapes become less and less significant. We show the whole process here for the record nonetheless.

## 6. Conclusion

In this paper, we studied the well posedness of a mathematical model of phosphorus uptake by plant roots, governed by a quasilinear convection-diffusion equation with a nonlinear boundary condition. We proved existence and uniqueness of solutions to the problem in Hölder spaces, assuming sufficient regularity of the data.

Then, we formulated a shape optimization problem to increase the amount of absorbed phosphorus by changing the shape of the root. The sensitivity analysis was performed using classical tools of shape optimization. The adjoint method was used to produce a gradient ascent algorithm in order to maximize the objective function.

A numerical example in two spatial dimensions with an elliptical initial shape was presented. This example shows that maximizing root surface area to volume ratio is indeed an essential component of root uptake efficiency. The resulting shape is evocative of the branching structure of plant root systems.

Future work could consist in coupling a similar shape sensitivity analysis with an explicit geometry root system growth model, in order to study and improve the efficiency of different types of root systems regarding nutrient and water uptake in heterogeneous soils.

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