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.

Keywords quasilinear parabolic equations; regularity estimates; phosphorus uptake; plant roots; shape optimization

Mathematics Subject Classification (2000) 35K20, 35K55

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.
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 environement. Moreoever, 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 Doussan et al. (1998), Roose et al. (2001) and Mollier et al. (2008). 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 domain, delimited by the root surface and the domain boundaries. Let Γ_1 be the boundary representing the root surface and $\Gamma_2 = \partial\Omega \setminus \Gamma_1$.

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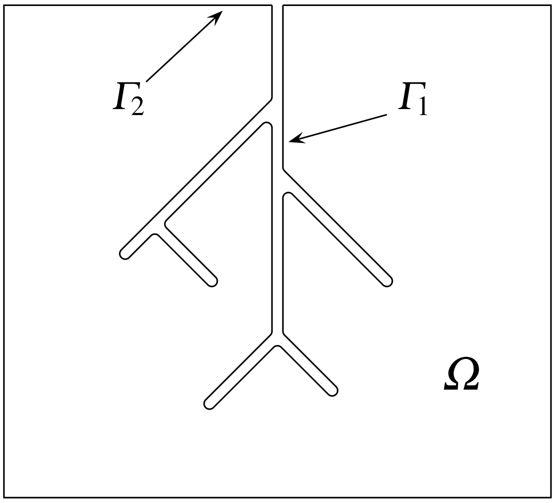

Fig. 1 Configuration of the domain

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:

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

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,
- θ is the volumetric water content,
- $\mathbf{q}$ is the groundwater flow,
- φ 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 (McGechan and Lewis 2002), defined by:

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

- 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 (Barber 1984), given by:

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

- R represents additional optional source/sink terms to the system. We will only consider source terms, such as fertilizer application,
- α is a parameter we introduce in order to obtain sufficient regularity of the boundary condition in the case $\Gamma_1 \cap \Gamma_2 \neq 0$: $\alpha \in C^2(\partial\Omega)$ such that for $x \in \partial\Omega$

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

We do not restrict ourselves to considering explicit forms for φ or h: we only use general properties of these functions throughout this paper.
Since φ is defined on $[0,+\infty[$, we consider positive solutions of problem (1.1).
The paper is organized as follows: we first discuss existence and uniqess 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.

For simplicity and clarity, we only take α into account while proving existence and uniqueness of the solution, and we drop it later in the shape optimization study.

We begin by introducing some notations:

- S is the boundary of Ω,
- 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 $x\in\overline{\Omega}$.

Let us make the following assumptions:
hypotheses on S

$$S\in C^{2+\beta}, \tag{1.2}$$

hypotheses on c^0

$$\begin{aligned} &c^0\in C^{2+\beta}(\overline{\Omega}),\, c^0>0,\\ &\left(A\nabla c^0-\mathbf{q}c^0\right)\cdot\mathbf{n}+h(c^0)=0 \text{ on } \Gamma_1,\\ &\left(A\nabla c^0-\mathbf{q}c^0\right)\cdot\mathbf{n}=0 \text{ on } \Gamma_2, \end{aligned} \tag{1.3}$$

hypotheses on φ

$$\varphi\in C^3((0,+\infty)),\, \varphi'>0, \tag{1.4}$$

hypotheses on A

$$A\in C^{1+\beta/2,2+\beta}(\overline{Q}),\, A_m\geq A(t,x)\geq A_0>0 \text{ in } \overline{Q}, \tag{1.5}$$

hypotheses on θ

$$\theta\in C^{1+\beta/2,2+\beta}(\overline{Q}),\, \theta_m\geq \theta(t,x)\geq \theta_0>0 \text{ in } \overline{Q}, \tag{1.6}$$

hypotheses on R

$$R\in C^{1+\beta/2,2+\beta}(\overline{Q}),\, R<0 \text{ in } \overline{Q}, \tag{1.7}$$

hypotheses on $\mathbf{q}$

$$q_i\in C^{1+\beta/2,2+\beta}(\overline{Q}),\, i=1,..,d, \tag{1.8}$$

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

$$h\in C^2(\mathbb{R}),\, h(0)=0,\, \|h\|_{L^\infty(\mathbb{R})}+\|h'\|_{L^\infty(\mathbb{R})}+\|h''\|_{L^\infty(\mathbb{R})}\leq C_h. \tag{1.9}$$

Here and in the sequel,

$$\beta\in(0,1). \tag{1.10}$$

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 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

$$\hat{c}(t,x) := \delta e^{-Kt}\hat{c}_0(x), \quad (t,x) \in Q, \tag{2.1}$$

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

$$A_0 \frac{\partial \hat{c}_0}{\partial n} < -\|\mathbf{q}\|_{L^\infty(Q)}\hat{c}_0(x) - (h'(0)+1)\hat{c}_0(x) \quad \forall x \in S, \tag{2.2}$$

and

$$0 < \hat{c}_0(x) < 1 \quad \forall x \in \overline{\Omega}. \tag{2.3}$$

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

$$\begin{cases} \theta \hat{c}_t - \operatorname{div}\left(A\nabla\hat{c} - \mathbf{q}\hat{c}\right) + R + \theta_t \hat{c} < 0 \text{ in } Q, \\ A\dfrac{\partial \hat{c}}{\partial n} < (\mathbf{q}\cdot\mathbf{n})\hat{c} - \alpha h(\hat{c}) & \text{on } S_T, \\ \hat{c}(0,x) < c^0(x) & \text{in } \overline{\Omega}. \end{cases} \tag{2.4}$$

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

$$(\theta + \varphi'(\hat{c}))\hat{c}_t - \operatorname{div}\left(A\nabla\hat{c} - \mathbf{q}\hat{c}\right) + R + \theta_t \hat{c} < 0 \quad \text{in} \quad Q. \tag{2.5}$$

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

Theorem 1 (Friedman (1964), 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 $F(t,x,p,p_i,p_{ij})$ $(i,j = 1,...,d)$ 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*

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

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

If

$$\begin{cases} \dfrac{\partial v}{\partial t} > F\left(t,x,v,\dfrac{\partial v}{\partial x_i},\dfrac{\partial^2 v}{\partial x_i \partial x_j}\right) & \text{in } Q, \\ \dfrac{\partial w}{\partial t} \leq F\left(t,x,w,\dfrac{\partial w}{\partial x_i},\dfrac{\partial^2 w}{\partial x_i \partial x_j}\right) & \text{in } Q, \\ v(0,x) > w(0,x) & \text{on } \overline{\Omega}, \\ \dfrac{\partial v}{\partial n} + \gamma(t,x,v) > \dfrac{\partial w}{\partial n} + \gamma(t,x,w) & \text{on } S_T, \end{cases} \tag{2.6}$$

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

We have

$$\begin{cases} c_t = (\theta + \varphi'(c))^{-1}(\operatorname{div}\left(A\nabla c - \mathbf{q}c\right) - R) - \theta_t c & \text{in} \quad [0,T'] \times \Omega, \\ A\nabla c \cdot \mathbf{n} = (\mathbf{q}\cdot\mathbf{n})c - \alpha h(c) & \text{on} \quad [0,T'] \times S, \end{cases} \tag{2.7}$$

and

$$\begin{cases} \hat{c}_t < (\theta + \varphi'(\hat{c}))^{-1}(\operatorname{div}\left(A\nabla\hat{c} - \mathbf{q}\hat{c}\right) - R) - \theta_t \hat{c} & \text{in} \quad [0,T'] \times \Omega, \\ A\nabla\hat{c} \cdot \mathbf{n} < (\mathbf{q}\cdot\mathbf{n})\hat{c} - \alpha h(\hat{c}) & \text{on} \quad [0,T'] \times S. \end{cases} \tag{2.8}$$

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 (1.4), (1.5), (1.6), (1.7) and (1.8).

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

$$c > \hat{c} \geq \delta e^{-KT} \min_{x\in\overline{\Omega}} \hat{c}_0(x) > 0 \quad \text{in} \quad [0,T'] \times \Omega. \tag{2.9}$$

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 $T' = \max\{t \in [0,T] \mid c \geq \varepsilon$ in $[0,T'] \times \overline{\Omega}\}$. Note that the lower bound is independent of the choice of ε. Then, it is easy to see that if we take ε 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

$$c > \delta e^{-KT} \min_{x\in\overline{\Omega}} \hat{c}_0(x) > 0 \quad \text{in} \quad Q. \tag{2.10}$$

• Estimate from above:

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

$$A_0 \frac{\partial \check{c}_0}{\partial n} > \|\mathbf{q}\|_{L^\infty(Q)} \check{c}_0(x) \quad \forall x \in S, \tag{2.11}$$

and

$$\|c^0\|_{L^\infty(\Omega)} < \check{c}_0(x) < \|c^0\|_{L^\infty(\Omega)} + 1 \quad \forall x \in \overline{\Omega}. \tag{2.12}$$

Let us define

$$\check{c}(t,x) := e^{\lambda t} \check{c}_0(x), \quad (t,x) \in Q, \tag{2.13}$$

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

$$\theta \check{c}_t - \operatorname{div}\left(A\nabla\check{c} - \mathbf{q}\check{c}\right) + R + \theta_t \check{c} > 0 \quad \text{in} \quad Q, \tag{2.14}$$

which means that

$$(\theta + \varphi'(\check{c}))\check{c}_t - \operatorname{div}\left(A\nabla\check{c} - \mathbf{q}\check{c}\right) + R + \theta_t \check{c} > 0 \quad \text{in} \quad Q. \tag{2.15}$$

We have

$$\begin{cases} c_t = (\theta + \varphi'(c))^{-1}(\operatorname{div}\left(A\nabla c - \mathbf{q}c\right) - R) - \theta_t c & \text{in} \quad Q, \\ A\nabla c \cdot \mathbf{n} = (\mathbf{q}\cdot\mathbf{n})c - \alpha h(c) & \text{on} \quad S_T, \end{cases} \tag{2.16}$$

and

$$\begin{cases} \check{c}_t > (\theta + \varphi'(\check{c}))^{-1}(\operatorname{div}\left(A\nabla\check{c} - \mathbf{q}\check{c}\right) - R) - \theta_t \check{c} & \text{in} \quad Q, \\ A\nabla\check{c} \cdot \mathbf{n} > (\mathbf{q}\cdot\mathbf{n})\check{c} - \alpha h(\check{c}) & \text{on} \quad S_T. \end{cases} \tag{2.17}$$

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

$$0 < c_{min} \leq c(t,x) \leq c_{max}, \quad (t,x) \in Q. \tag{2.18}$$

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

In this section, we prove the uniqueness of solutions of problem (1.1) in the space $C^{1,2}(\overline{Q})$.
Let c_1, c_2 be two solutions of (1.1) belonging to $C^{1,2}(\overline{Q})$. From section 2, we know that

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

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

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

We use that $\theta_t \in L^\infty(\Omega \times (0,T))$ (see (1.6)), $\varphi''(c_1) \in L^\infty(\Omega \times (0,T))$ (thanks to (1.4) and (3.1)) and $\mathbf{q} \in L^\infty(\Omega \times (0,T))$.
We obtain:

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

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

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

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

Using that

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

we deduce that

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

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

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

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

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

where K'_ε does not depend on K_ε.

• 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,

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

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

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

Putting this together with (3.4) and using (1.4), (1.5) and (1.6), we find

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

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 (1.10).
In order to apply an existence and uniqueness theorem we need to define a new problem by truncating the function φ:

Let us define φ_M as follows, with $M := \begin{pmatrix} M_1 \\ M_2 \end{pmatrix}, 0 < M_1 < M_2$:

$$\begin{cases}
\varphi_M(c) = \varphi(c) \text{ for } M_1 \leq c \leq M_2, \\
\varphi_M(c) = -\varepsilon_M \text{ for } c \leq -\varepsilon_M, \\
\varphi_M(c) = \varphi(M_2)+\varepsilon_M \text{ for } c \geq M_2+\varepsilon_M, \\
\varphi_M \in C^3([-\varepsilon_M, M_1]\cup[M_2, M_2+\varepsilon_M]), \\
\varphi_M' \geq 0,
\end{cases}$$

for some $\varepsilon_M > 0$.
It is clear that such φ_M exists. Note, in particular, that $\varphi_M'(c) = \varphi_M''(c) = \varphi_M'''(c) = 0$ for $|c| > M_2+\varepsilon_M$ and that φ_M and its derivatives of up to order three are bounded.

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

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

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:

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

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:

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

Using the chain rule yields:

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

We obtain:

$$\begin{aligned} \partial_t y - A\sum_i \left[k_{x_ix_i} + k_y y_{x_ix_i} + k_{yx_i}y_{x_i} + k_{x_iy}y_{x_i} + k_{yy}y_{x_i}^2\right] \\ -\sum_i \left[A_{x_i}k_{x_i} + A_{x_i}k_y y_{x_i} - kq_{i_{x_i}} - q_i k_{x_i} - q_i k_y y_{x_i}\right] + R = 0. \end{aligned}$$

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

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

Using the chain rule again yields:

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

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

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

with

$$\begin{cases} a_{ij} = 0 \;\; \text{for} \;\; i\neq j, \\ a_{ii} = Ak_y, \\ \;\; b = -A\sum_i \left[k_{x_ix_i} + k_{yx_i}y_{x_i} + k_{x_iy}y_{x_i} + k_{yy}y_{x_i}^2\right] \\ \qquad -\sum_i \left[A_{x_i}k_{x_i} + A_{x_i}k_y y_{x_i} - kq_{i_{x_i}} - q_i k_{x_i} - q_i k_y y_{x_i}\right] + R, \\ \;\psi = \sum_i (Ak_{x_i} - q_i k)cos(\mathbf{n},x_i) + \alpha h(k). \end{cases} \tag{4.4}$$

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

Theorem 2 (Ladyzhenskaya et al. (1968), 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,*

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

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

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

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

There exists $\nu, \mu > 0$ *such that for* $(t,x) \in \overline{Q}$ *,* $|y| \leq N$ *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:*

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

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

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

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

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

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

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

$$-yb(x,t,y,p) = \sum_i \left[Ak_{x_ix_i}y + A_{x_i}k_{x_i}y - kq_{i_{x_i}}y - q_ik_{x_i}y \right] - Ry$$
$$+ A\sum_i \left[k_{yx_i}p_iy + k_{x_iy}p_iy + k_{yy}p_i^2 y \right] + \sum_i \left[A_{x_i}k_yp_iy - q_ik_yp_iy \right].$$

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

$$\begin{aligned} k_{x_ix_j} =& -\frac{\theta_{x_ix_j}k}{\theta+\varphi_M'(k)} + \frac{2\theta_{x_i}\theta_{x_j}k}{(\theta+\varphi_M'(k))^2} - \frac{\theta_{x_i}\theta_{x_j}\varphi_M''(k)k^2}{(\theta+\varphi_M'(k))^3} \\ &+ \frac{\theta^0_{x_ix_j}c^0+\theta^0_{x_i}c^0_{x_j}+(\theta^0+\varphi_M'(c^0))c^0_{x_ix_j}+(\theta^0_{x_j}+\varphi_M''(c^0)c^0_{x_j})c^0_{x_i}}{\theta+\varphi_M'(k)} \\ &- \left(\theta^0_{x_i}c^0+(\theta^0+\varphi_M'(c^0))c^0_{x_i}\right) \\ &\left(\frac{\theta_{x_j}}{(\theta+\varphi_M'(k))^2} + \frac{\varphi_M''(k)(\theta^0_{x_i}c^0+(\theta^0+\varphi_M'(c^0))c^0_{x_i})}{(\theta+\varphi_M'(k))^3} - \frac{\varphi_M''(k)\theta_{x_i}k}{(\theta+\varphi_M'(k))^3}\right). \end{aligned}$$

We have $\theta_0 \le \theta(t,x)+\varphi_M'(k) < +\infty$. 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 θ, A, θ^0, c^0 and their space derivatives of up to order two are bounded , it follows that there exists $c_{3a}, c_{3b} \ge 0$ such that for arbitrary y

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

Remaining terms not involving p are handled similarly.

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

$$k_{yx_i} = \frac{-\theta_{x_i}}{(\theta+\varphi_M'(k))^2} + \frac{\theta_{x_i}\varphi_M''(k)k}{(\theta+\varphi_M'(k))^3} - \frac{\varphi_M''(k)\left(\theta^0_{x_i}c^0+(\theta^0+\varphi_M'(c^0))c^0_{x_i}\right)}{(\theta+\varphi_M'(k))^3},$$

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

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

– The term $Ak_{yy}p_i^2y$ 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 $c_6 \ge 0$ such that for arbitrary y

$$|Ak_{yy}p_i^2y| \le c_6p^2 \quad \text{for} \quad (t,x)\in\overline{Q}.$$

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, thus it is clear that these conditions are verified.

Proof of (4.8). We have

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

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:

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

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

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

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 section 2. Moreover, one can easily see that c_M can be bounded independently of M: $\forall\, M = \begin{pmatrix} M_1 \\ M_2 \end{pmatrix}$, $0 < M_1 < M_2$,

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

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 section 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 by Sokolowski and Zolesio (1992), Haslinger and Makinen (2003) and Henrot and Pierre (2005) to find root shapes that increase the amount of absorbed P. More specifically, we want to deform Ω so as to maximize the shape functional

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

where $|\Omega| =$ a given constant.
It is assumed that A and $\mathbf{q}$ are constants for simplicity.
We first calculate the material and shape derivatives of c with respect to the domain:
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 $T_s(\mathbf{V}) = Id + s\mathbf{V}$ and let c_s be the unique solution of

$$\begin{cases} \partial_t(\theta c_s + \varphi(c_s)) = \text{div}\left(A\nabla c_s - \mathbf{q}c_s\right) - R & \text{in} \quad I\times\Omega_s, \\ h(c_s) = -\left(A\nabla c_s - \mathbf{q}c_s\right)\cdot\mathbf{n} & \text{on} \quad I\times\Gamma_{1,s}, \\ 0 = -\left(A\nabla c_s - \mathbf{q}c_s\right)\cdot\mathbf{n} & \text{on} \quad I\times\Gamma_{2,s} = I\times(\partial\Omega\setminus\Gamma_{1,s}), \\ c_s(0,x) = z(x) & \in H^1(\mathbb{R}^n). \end{cases} \tag{5.1}$$

We first determine the form of $\dot{c}$, the material derivative of c, which is the derivative of $s \to c_s\circ T_s$ at $s = 0$.
For s small enough, c_s satisfies

$$\begin{aligned} \int_0^T \int_{\Omega_s} -(\theta c_s + \varphi(c_s))\partial_t\Phi + (A\nabla c_s - \mathbf{q}c_s)\cdot\nabla\Phi + R\Phi \\ = \int_{\Omega_s}(\theta z + \varphi(z))\Phi(0,x)dx - \int_0^T\int_{\Gamma_{1,s}} \Phi h(c_s)\sigma dt, \end{aligned} \tag{5.2}$$

for all $\Phi\in H^1(\Omega_s)$ such that

$$\Phi(T,\cdot) = 0.$$

We use the change of variable $x = T_s(\mathbf{V})(X)$ and introduce $c^s = c_s\circ T_s(\mathbf{V})$ and $\Phi^s_{\mathbf{V}} = \Phi\circ T_s(\mathbf{V})$. The Jacobian of the transformation is then $\det(D(T_s(\mathbf{V})) = \det(DT_s)$.

Using this change of variable in (5.2) leads to

$$\begin{aligned}
&\int_0^T \int_\Omega -(\theta c^s + \varphi(c^s))\partial_t \Phi_{\mathbf{V}}^s |\det(DT_s)| \\
&+ \int_0^T \int_\Omega (A(^*D(T_s))^{-1}\nabla c^s - \mathbf{q}c^s) \cdot (^*D(T_s))^{-1}\nabla \Phi_{\mathbf{V}}^s |\det(DT_s)| \\
&+ \int_0^T \int_\Omega R \circ T_s \Phi_{\mathbf{V}}^s |\det(DT_s)| \\
&= \int_\Omega (\theta z \circ T_s + \varphi(z \circ T_s))\Phi_{\mathbf{V}}^s(0,x)|\det(DT_s)| \\
&- \int_0^T \int_{\Gamma_1} \Phi_{\mathbf{V}}^s h(c^s)|\det(DT_s)| \quad \|(^*D(T_s))^{-1}(\mathbf{n})\|,
\end{aligned} \tag{5.3}$$

with

$$\Phi(T,\cdot) = 0.$$

As Φ is any element in $H^1(\Omega_s)$, $\Phi_{\mathbf{V}}^s$ describes $H^1(\Omega)$. Then using (5.3) leads to

$$\begin{aligned}
&\int_0^T \int_\Omega -(\theta c^s + \varphi(c^s))\partial_t \Phi |\det(DT_s)| \\
&+ \int_0^T \int_\Omega (A(^*D(T_s))^{-1}\nabla c^s - \mathbf{q}c^s) \cdot (^*D(T_s))^{-1}\nabla \Phi |\det(DT_s)| \\
&+ \int_0^T \int_\Omega R \circ T_s \Phi |\det(DT_s)| = \int_\Omega (\theta z \circ T_s + \varphi(z \circ T_s))\Phi(0,x)|\det(DT_s)| \\
&- \int_0^T \int_{\Gamma_1} \Phi h(c^s)|\det(DT_s)| \quad \|(^*D(T_s))^{-1}(\mathbf{n})\|.
\end{aligned} \tag{5.4}$$

Furthermore, using (1.1) gives

$$\begin{aligned}
&\int_0^T \int_\Omega -(\theta c + \varphi(c))\partial_t \Phi + (A\nabla c - \mathbf{q}c) \cdot \nabla \Phi \\
&+ \int_0^T \int_\Omega R\Phi = \int_\Omega (\theta z + \varphi(z)\Phi(0,x) - \int_0^T \int_{\Gamma_1} \Phi h(c).
\end{aligned} \tag{5.5}$$

Subtracting (5.3) to (5.4), dividing by s and letting s go to 0 leads to

$$\begin{aligned}
&\int_0^T \int_\Omega -(\theta \dot{c} + \varphi'(c)\dot{c} + \theta c \operatorname{div} \mathbf{V} + \varphi(c) \operatorname{div} \mathbf{V})\partial_t \Phi \\
&+ \int_0^T \int_\Omega A(\nabla \dot{c} + (\operatorname{div} \mathbf{V} -^* DV - DV)\nabla c) \cdot \nabla \Phi \\
&+ \int_0^T \int_\Omega -\mathbf{q} \cdot (\dot{c} - c^* DV + c \operatorname{div} \mathbf{V})\nabla \Phi + \int_0^T \int_\Omega (\nabla R \cdot \mathbf{V} + R \operatorname{div} \mathbf{V})\Phi \\
&= \int_\Omega (\theta \nabla z \cdot \mathbf{V} + \theta z \operatorname{div} \mathbf{V} + \nabla(\varphi \circ z) \cdot \nabla \mathbf{V} + \varphi(z) \operatorname{div} \mathbf{V})\Phi(0,x) \\
&- \int_0^T \int_{\Gamma_1} (h'(c)\dot{c} + h(c)(\operatorname{div} \mathbf{V} - DV\mathbf{n} \cdot \mathbf{n}))\Phi.
\end{aligned} \tag{5.6}$$

Integrating by parts the first term gives

$$\begin{aligned}
&\int_0^T \int_\Omega \frac{\partial}{\partial t}(\theta \dot{c} + \varphi'(c)\dot{c} + \theta c \,\mathrm{div}\,\mathbf{V} + \varphi(c)\,\mathrm{div}\,\mathbf{V})\Phi \\
&+ \int_0^T \int_\Omega A(\nabla \dot{c} + (\mathrm{div}\,\mathbf{V} -^* DV - DV)\nabla c) \cdot \nabla \Phi \\
&+ \int_0^T \int_\Omega -\mathbf{q} \cdot \big(\dot{c} - c^* DV + c\,\mathrm{div}\,\mathbf{V}\big)\nabla \Phi + \int_0^T \int_\Omega (\nabla R \cdot \mathbf{V} + R\,\mathrm{div}\,\mathbf{V})\Phi \\
&= \int_\Omega \Big(\theta \nabla z \cdot \mathbf{V} - \big(\theta + \varphi'(c(0,x))\big)\dot{c}(0,x) + \nabla(\varphi \circ z) \cdot \nabla \mathbf{V}\Big)\Phi(0,x) \\
&- \int_0^T \int_{\Gamma_1} (h'(c)\dot{c} + h(c)(\mathrm{div}\,\mathbf{V} - DV\mathbf{n} \cdot \mathbf{n}))\Phi.
\end{aligned}$$

Integrating by parts the following two terms leads to

$$\begin{aligned}
&\int_0^T \int_\Omega \frac{\partial}{\partial t}\big(\theta \dot{c} + \varphi'(c)\dot{c} + \theta c \,\mathrm{div}\,\mathbf{V} + \varphi(c)\,\mathrm{div}\,\mathbf{V}\big)\Phi \\
&- \int_0^T \int_\Omega A\big(\Delta \dot{c} + \mathrm{div}(\mathrm{div}\,\mathbf{V} -^* DV - DV)\nabla c\big)\Phi \\
&+ \int_0^T \int_{\partial\Omega} A\big(\frac{\partial \dot{c}}{\partial n} + (\mathrm{div}\,\mathbf{V} -^* DV - DV)\nabla c \cdot \mathbf{n}\big)\Phi \\
&+ \int_0^T \int_\Omega \mathbf{q} \cdot \big(\nabla \dot{c} - c\nabla(\mathrm{div}\,\mathbf{V}) + \mathrm{div}\,\mathbf{V}\nabla c\big)\Phi + \\
&\int_0^T \int_\Omega \big(-DV\mathbf{q} \cdot \nabla c + c\,\mathrm{div}(DV\mathbf{q})\big)\Phi + \\
&+ \int_0^T \int_{\partial\Omega} \Big(-\dot{c}\mathbf{q} \cdot \mathbf{n} + DV(c\mathbf{q}) \cdot \mathbf{n} - \mathrm{div}\,\mathbf{V} c\mathbf{q} \cdot \mathbf{n}\Big)\Phi + \int_0^T \int_\Omega (\nabla R \cdot \mathbf{V} + R\,\mathrm{div}\,\mathbf{V})\Phi \\
&= \int_\Omega \Big(\theta \nabla z \cdot \mathbf{V} - \big(\theta + \varphi'(c(0,x))\big)\dot{c}(0,x) + \nabla(\varphi \circ z) \cdot \nabla \mathbf{V}\Big)\Phi(0,x) + \\
&- \int_0^T \int_{\Gamma_1} (h'(c)\dot{c} + h(c)(\mathrm{div}\,\mathbf{V} - DV\mathbf{n} \cdot \mathbf{n}))\Phi.
\end{aligned}$$

Finally, the equation verified by $\dot{c}$ in Q is

$$\begin{aligned}
&\frac{\partial}{\partial t}\big(\theta \dot{c} + \varphi'(c)\dot{c} + \theta c \,\mathrm{div}\,\mathbf{V} + \varphi(c)\,\mathrm{div}\,\mathbf{V}\big) \\
&-A\big(\Delta \dot{c} + \mathrm{div}(\mathrm{div}\,\mathbf{V} -^* DV - DV)\nabla c\big) \\
&+\mathbf{q} \cdot \big(\nabla \dot{c} - c\nabla(\mathrm{div}\,\mathbf{V}) + \mathrm{div}\,\mathbf{V}\nabla c\big) - \\
&-DV\mathbf{q} \cdot \nabla c + c\,\mathrm{div}(DV\mathbf{q}) = -\nabla R \cdot \mathbf{V} - R\,\mathrm{div}\,\mathbf{V},
\end{aligned} \tag{5.7}$$

with boundary conditions

$$\begin{cases}
A\big(\frac{\partial \dot{c}}{\partial n} + (\mathrm{div}\,\mathbf{V} -^* DV - DV)\nabla c \cdot \mathbf{n}\big) - \dot{c}\mathbf{q} \cdot \mathbf{n} + DV(c\mathbf{q}) \cdot \mathbf{n} - \mathrm{div}\,\mathbf{V} c\mathbf{q} \cdot \mathbf{n} = \\
-h'(c)\dot{c} - h(c)(\mathrm{div}\,\mathbf{V} - DV\mathbf{n} \cdot \mathbf{n}) \quad \text{on} \quad I \times \Gamma_1, \\
A\big(\frac{\partial \dot{c}}{\partial n} + (\mathrm{div}\,\mathbf{V} -^* DV - DV)\nabla c \cdot \mathbf{n}\big) - \dot{c}\mathbf{q} \cdot \mathbf{n} + DV(c\mathbf{q}) \cdot \mathbf{n} - \\
-\mathrm{div}\,\mathbf{V} c\mathbf{q} \cdot \mathbf{n} = 0 \quad \text{on} \quad I \times \Gamma_2,
\end{cases} \tag{5.8}$$

and initial value

$$(\theta + \varphi'(c(0,x)))\dot{c}(0,x) = \theta \nabla z \cdot \mathbf{V} + \nabla(\varphi \circ z) \cdot \nabla \mathbf{V}. \tag{5.9}$$

Using the original equation satisfied by c, we obtain

$$\begin{aligned}\frac{\partial}{\partial t}\big(\theta\dot{c}+\varphi'(c)\dot{c}\big)-A\Delta\dot{c}+\mathbf{q}\cdot\big(\nabla\dot{c}-c\nabla(\operatorname{div}\mathbf{V})\big)\\ -A\nabla(\operatorname{div}\mathbf{V})\cdot\nabla c-DV\mathbf{q}\cdot\nabla c+c\operatorname{div}(DV\mathbf{q})\\ +A\big(\operatorname{div}({}^*DV+DV)\nabla c\big)=-\nabla R\cdot\mathbf{V}\quad\text{in}\quad Q,\end{aligned}\tag{5.10}$$

with boundary conditions

$$\begin{cases}A\big(\frac{\partial\dot{c}}{\partial n}-({}^*DV+DV)\nabla c\cdot\mathbf{n}\big)-\dot{c}\mathbf{q}\cdot\mathbf{n}\\ +DV(c\mathbf{q})\cdot\mathbf{n}=-h'(c)\dot{c}+h(c)DV\mathbf{n}\cdot\mathbf{n}\quad\text{on}\quad I\times\Gamma_1,\\ A\big(\frac{\partial\dot{c}}{\partial n}-({}^*DV+DV)\nabla c\cdot\mathbf{n}\big)-\dot{c}\mathbf{q}\cdot\mathbf{n}+DV(c\mathbf{q})\cdot\mathbf{n}\\ =0\quad\text{on}\quad I\times\Gamma_2,\end{cases}\tag{5.11}$$

and initial value

$$(\theta+\varphi'(c(0,x)))\dot{c}(0,x)=\theta\nabla z\cdot\mathbf{V}+\nabla(\varphi\circ z)\cdot\nabla\mathbf{V}.\tag{5.12}$$

Let us now denote by c' the derivative of c with respect to the domain: $c'=\dot{c}-\nabla c\cdot\mathbf{V}$.

The equation satisfied by c' is

$$\frac{\partial}{\partial t}\big(\theta c'+\varphi'(c)c'\big)-A\Delta c'+\mathbf{q}\cdot\nabla c'=0\quad\text{in}\quad Q,\tag{5.13}$$

with boundary conditions

$$\begin{cases}A\frac{\partial c'}{\partial n}-c'\mathbf{q}\cdot\mathbf{n}+h'(c)c'=\big(-A\frac{\partial^2 c}{\partial n^2}-\frac{\partial h(c)}{\partial n}+\nabla c\cdot\mathbf{q}\big)(\mathbf{V}\cdot\mathbf{n})\\ +A\nabla_T(\mathbf{V}\cdot\mathbf{n})\cdot\nabla_T c-\nabla_T(c\mathbf{V}\cdot\mathbf{n})\cdot\mathbf{q}\quad\text{on}\quad I\times\Gamma_1,\\ A\frac{\partial c'}{\partial n}-c'\mathbf{q}\cdot\mathbf{n}=\big(-A\frac{\partial^2 c}{\partial n^2}+\nabla c\cdot\mathbf{q}\big)(\mathbf{V}\cdot\mathbf{n})\\ +A\nabla_T(\mathbf{V}\cdot\mathbf{n})\cdot\nabla_T c-\nabla_T(c\mathbf{V}\cdot\mathbf{n})\cdot\mathbf{q}\quad\text{on}\quad I\times\Gamma_2,\end{cases}\tag{5.14}$$

and initial value

$$c'(0,x)=0,\tag{5.15}$$

where ∇_T is the tangential part of the gradient.

Now, consider the derivative of the functional J at Ω in the direction $\mathbf{V}$:

$$dJ(c,\mathbf{V})=\int_0^T\left(\int_{\Gamma_1}h'(c)c'+\int_{\Gamma_1}Hh(c)(\mathbf{V}\cdot\mathbf{n})+\int_{\Gamma_1}h'(c)\frac{\partial c}{\partial n}(\mathbf{V}\cdot\mathbf{n})\right),\tag{5.16}$$

where H is the mean curvature of the boundary of the domain.

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, we use the adjoint state technique. Let us introduce p the solution to the following adjoint state problem:

$$\begin{cases}-(\theta+\varphi'(c))\partial_t p-\operatorname{div}(A\nabla p)-\mathbf{q}\cdot\nabla p=0 & \text{in}\ \ Q,\\ (A\nabla p)\cdot\mathbf{n}+h'(c)p=h'(c) & \text{on}\ \ I\times\Gamma_1,\\ (A\nabla p)\cdot\mathbf{n}=0 & \text{on}\ \ I\times\Gamma_2,\\ p(T,x)=0 & \text{in}\ \ \Omega?\end{cases}\tag{5.17}$$

Multiplying by c' and integrating over Q yields:

$$-\int_0^T\int_\Omega(\theta+\varphi'(c))\partial_t pc'-\int_0^T\int_\Omega-\operatorname{div}(A\nabla p)c'-\int_0^T\int_\Omega\mathbf{q}\cdot\nabla pc'=0.\tag{5.18}$$

Successive integrations by parts lead to

$$\begin{aligned}&\int_0^T\int_\Omega \partial_t(\theta c' + \varphi'(c)c')p - \int_\Omega (\theta + \varphi'(c(x,T)))c'(x,T)p(x,T) + \int_\Omega (\theta + \varphi'(c(x,0)))c'(x,0)p(x,0)\\ &+\int_0^T\int_\Omega A\nabla c'\cdot\nabla p - \int_0^T\int_\Gamma Ac'\frac{\partial p}{\partial n} + \int_0^T\int_\Omega p\,\mathrm{div}(\mathbf{q}c') - \int_0^T\int_\Gamma c'p\mathbf{q}\cdot\mathbf{n} = 0,\end{aligned} \tag{5.19}$$

and finally

$$\begin{aligned}&\int_0^T\int_\Omega \partial_t(\theta c' + \varphi'(c)c')p - \int_0^T\int_\Omega \mathrm{div}(A\nabla c')p + \int_0^T\int_\Gamma A\frac{\partial c'}{\partial n}p - \int_0^T\int_\Gamma Ac'\frac{\partial p}{\partial n}\\ &+\int_0^T\int_\Omega p\,\mathrm{div}(\mathbf{q}c') - \int_0^T\int_\Gamma c'p\mathbf{q}\cdot\mathbf{n} = 0.\end{aligned} \tag{5.20}$$

On another hand, recall that

$$\partial_t(\theta c' + \varphi'(c)c') - \mathrm{div}(A\nabla c' - \mathbf{q}c') = 0 \quad \text{in} \quad Q. \tag{5.21}$$

Using (5.21) in (5.20) gives

$$\int_0^T\int_\Gamma A\frac{\partial c'}{\partial n}p - \int_0^T\int_\Gamma Ac'\frac{\partial p}{\partial n} - \int_0^T\int_\Gamma c'p\mathbf{q}\cdot\mathbf{n} = 0.$$

Considering the boundary conditions satisfied by p, it follows that

$$\int_0^T\int_\Gamma A\frac{\partial c'}{\partial n}p + \int_0^T\int_{\Gamma_1} h'(c)c'p - \int_0^T\int_\Gamma c'p\mathbf{q}\cdot\mathbf{n} = \int_0^T\int_{\Gamma_1} h'(c)c'. \tag{5.22}$$

We can now use (5.22) in equation (5.16) verified by dJ in order to get rid of c':

$$\begin{aligned}dJ(c,\mathbf{V}) &= \int_0^T\left(\int_{\Gamma_1} h'(c)c' + \int_{\Gamma_1} Hh(c)(\mathbf{V}\cdot\mathbf{n}) + \int_{\Gamma_1} h'(c)\frac{\partial c}{\partial n}(\mathbf{V}\cdot\mathbf{n})\right)\\ &= \int_0^T\left(\int_\Gamma A\frac{\partial c'}{\partial n}p + \int_{\Gamma_1} h'(c)c'p - \int_0^T\int_\Gamma c'p\mathbf{q}\cdot\mathbf{n} + \int_{\Gamma_1} Hh(c)(\mathbf{V}\cdot\mathbf{n}) + \int_{\Gamma_1} h'(c)\frac{\partial c}{\partial n}(\mathbf{V}\cdot\mathbf{n})\right)\\ &= \int_0^T\left(\int_\Gamma A\nabla_T c\cdot\nabla_T(\mathbf{V}\cdot\mathbf{n})p - A\frac{\partial^2 c}{\partial n^2}(\mathbf{V}\cdot\mathbf{n})p - \nabla_T(c\mathbf{V}\cdot\mathbf{n})\cdot\mathbf{q}p + \mathbf{q}\cdot\nabla c(\mathbf{V}\cdot\mathbf{n})p\right)\\ &\quad - \int_0^T\left(\int_{\Gamma_1} h'(c)\frac{\partial c}{\partial n}(\mathbf{V}\cdot\mathbf{n})p - (Hh(c) + h'(c)\frac{\partial c}{\partial n})(\mathbf{V}\cdot\mathbf{n})\right),\end{aligned} \tag{5.23}$$

where the last equality comes from using the boundary conditions satisfied by c'.

Now, note that

$$\begin{aligned}\int_\Gamma A\nabla_T c\cdot\nabla_T(\mathbf{V}\cdot\mathbf{n})p &= -\int_\Gamma \mathrm{div}_T(Ap\nabla_T c)(\mathbf{V}\cdot\mathbf{n})\\ &= -\int_\Gamma A\nabla_T p\cdot\nabla_T c(\mathbf{V}\cdot\mathbf{n}) - \int_\Gamma p\,\mathrm{div}_T(A\nabla_T c)(\mathbf{V}\cdot\mathbf{n}).\end{aligned} \tag{5.24}$$

On the other hand, we have

$$\begin{aligned}\mathrm{div}_T(A\nabla_T c) = A\Delta_T c &= A\Delta c - AH\frac{\partial c}{\partial n} - A\frac{\partial^2 c}{\partial n^2}\\ &= \partial_t(\theta c + \varphi(c)) + \mathrm{div}(\mathbf{q}c) - AH\frac{\partial c}{\partial n} - A\frac{\partial^2 c}{\partial n^2}.\end{aligned} \tag{5.25}$$

It follows that

$$\int_\Gamma A\nabla_T c\cdot\nabla_T(\mathbf{V}\cdot\mathbf{n})p = -\int_\Gamma A\nabla_T p\cdot\nabla_T c(\mathbf{V}\cdot\mathbf{n}) - \int_\Gamma \partial_t(\theta c+\varphi(c))p(\mathbf{V}\cdot\mathbf{n})$$
$$-\int_\Gamma \mathrm{div}(\mathbf{q}c)p(\mathbf{V}\cdot\mathbf{n}) + \int_\Gamma AH\frac{\partial c}{\partial n}p(\mathbf{V}\cdot\mathbf{n}) + \int_\Gamma A\frac{\partial^2 c}{\partial n^2}p(\mathbf{V}\cdot\mathbf{n}).$$

Finally,

$$dJ(c,\mathbf{V}) = -\int_0^T\left(\int_\Gamma A\nabla_\Gamma p\cdot\nabla_\Gamma c(\mathbf{V}\cdot\mathbf{n}) - \int_\Gamma c\nabla_T p\cdot\mathbf{q}(\mathbf{V}\cdot\mathbf{n}) + \int_\Gamma \partial_t(\theta c+\varphi(c))p(\mathbf{V}\cdot\mathbf{n})\right)$$
$$+\int_0^T\left(\int_\Gamma AH\frac{\partial c}{\partial n}p(\mathbf{V}\cdot\mathbf{n}) - \int_{\Gamma_1} h'(c)\frac{\partial c}{\partial n}(\mathbf{V}\cdot\mathbf{n})p + \int_{\Gamma_1} Hh(c)(\mathbf{V}\cdot\mathbf{n}) + \int_{\Gamma_1} h'(c)\frac{\partial c}{\partial n}(\mathbf{V}\cdot\mathbf{n})\right).$$

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. $\mathbf{V} = jn$. this brings

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

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 $\mathbf{n}$.

Numerical resolution of the state and adjoint equations in two spatial dimensions is carried out using the free finite element software FreeFEM++. 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 this example are as follows:

- $F_m = 0.282\ \mu\mathrm{mol\,cm^{-2}\,d^{-1}}$, $K_m = 5.8\times10^{-3}\ \mu\mathrm{mol\,cm^{-3}}$,
- $\kappa = 6.15$, $b = 0.72$,
- $\theta = 0.35\ \mathrm{cm^3\,cm^{-3}}$,
- $A = 0.102\ \mathrm{cm^2\,d^{-1}}$,
- $c^0 = 2.9\times10^{-3}\ \mu\mathrm{mol\,cm^{-3}}$,
- $\mathbf{q} = 0, R = 0$.
- The initial shape is an ellipse of diameters 1.33 cm and 2.66 cm.

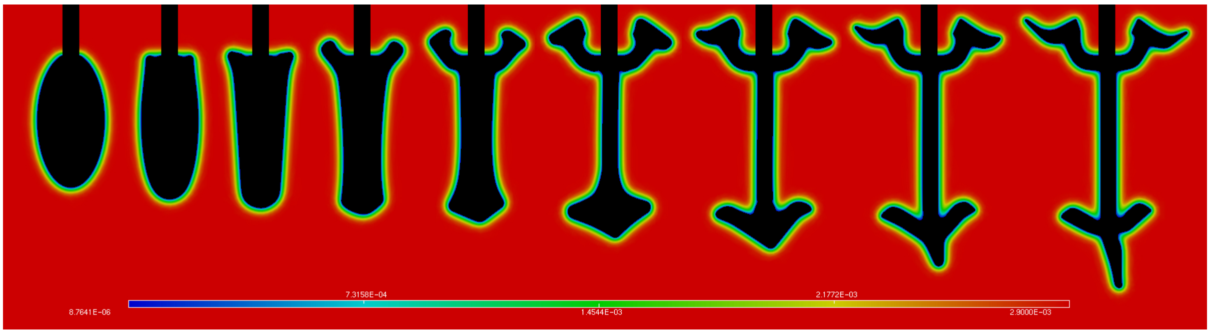

Fig. 2 Snapshots of the domain and P concentration at different steps of the shape optimization process

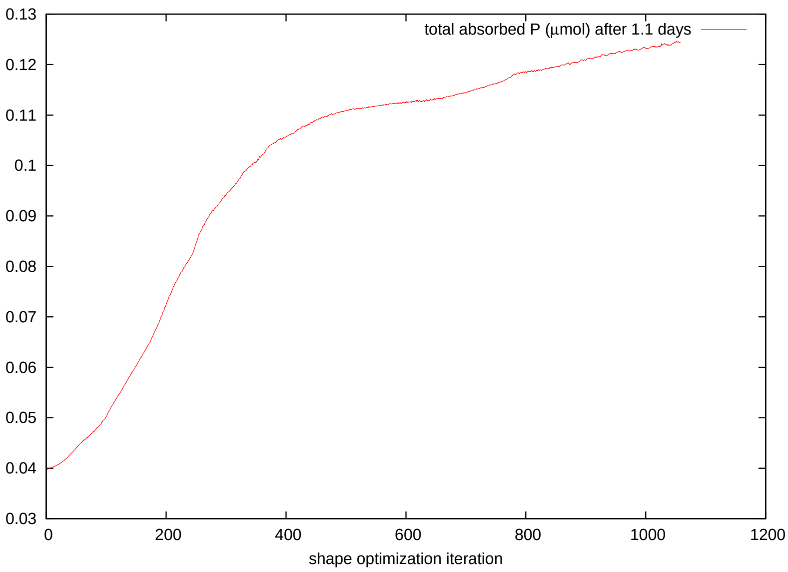

Fig. 3 Evolution of the total amount of absorbed P during the optimization process

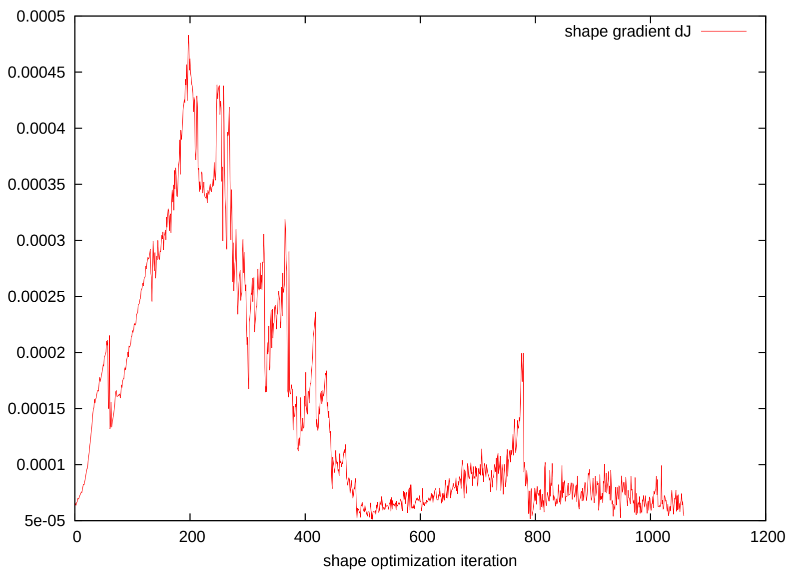

Fig. 4 Evolution of the shape gradient dJ during the optimization process

6 Conclusion

As expected, this example shows that maximizing root surface area to volume ratio is indeed an essential component of root uptake efficiency. 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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