Modelling bioremediation of polluted soils in unsaturated condition and its effec on the soil hydraulic properties

53 (2008) APPLICATIONS OF MATHEMATICS No. 5, 409–432

MODELLING BIOREMEDIATION OF POLLUTED SOILS IN UNSATURATED CONDITION AND ITS EFFECT ON THE SOIL HYDRAULIC PROPERTIES

Iacopo Borsi, Angiolo Farina, Antonio Fasano,
Mario Primicerio, Firenze

Dedicated to Jürgen Sprekels on the occasion of his 60th birthday

Abstract. We study the unsaturated flow of an incompressible liquid carrying a bacterial population through a porous medium contaminated with some pollutant. The biomass grows feeding on the pollutant and affecting at the same time all the physics of the flow. We formulate a mathematical model in a one-dimensional setting and we prove an existence theorem for it. The so-called fluid media scaling approach, often used in the literature, is discussed and its limitations are pointed out on the basis of a specific example.

Keywords: flows in porous media, continuous dependence on parameters

MSC 2000: 35B30, 76S05

1. Introduction

The topic of this paper is the analysis of the flow through porous media contaminated by some chemical species in presence of a growing biomass feeding on the pollutant. In turn, the growing bacterial population affects the hydraulic properties of the medium.

We refer to a typical *column experiment*, i.e. a variably saturated sand-filled column, in presence of a substrate (the pollutant) and inoculated with a well-known bacterium. The biomass may distribute in water as suspension (*free biomass*) or attached to the soil grains (*attached biomass*).

The literature devoted to the experimental study of biomass transport in order to evaluate the biodegradation process of the soils or aquifers is very numerous. In particular, the general topic of bioremediation has been deeply investigated in search of a good mathematical model (see [1] and [6], for instance).

The biomass affects the hydraulic properties of the medium in several ways.

- The free biomass has an influence on the viscosity, density and surface tension of the liquid-cell system.
- The attached biomass reduces the volume available for the flow and the contact angle, thus influencing also capillarity.
- The permeability and the relative saturation of the medium are modified too by the presence of the biomass.

Such effects are well known and extensively described by many authors (see [5], [8], [9] and the reference therein).

Various modelling techniques have been developed to take into account such complex phenomena, for instance the so-called *fluid media scaling* (see [7]). We shall return to this point later on.

In [2] we defined a model for a macroscopic description of the problem and accounting for

- Variably saturated flow in the medium (Richard's equation), with:
  - Porosity depending on the volume fraction occupied by attached biomass.
  - Variable saturated permeability (since it depends on porosity).
  - Moisture content description based on mixture theory (i.e. considering mobile water and water stored into the attached biomass).
- Advection, diffusion and reaction equations for pollutant and biomass in water.
- Reaction equations for attached biomass and pollutant adsorbed on soil.

Numerical simulations have shown the qualitative consistency of the model.

In this paper we introduce a slightly different version (see Section 2) with more attention to the modification of the porosity accompanying the evolution of the biomass, with the aim of showing an existence theorem for the related mathematical problem (Section 3). We will confine to the case of unsaturated flows (saturated flows have been studied more extensively, see e.g. [6]). Finally, in Section 4 we discuss the consistency of the so-called *fluid media scaling* approach. The latter procedure is very convenient from the computational point of view (and it was used also in [2]), but there are caveats concerning its adoption, which will be pointed out by means of an explicit example.

2. The model

2.1. Physical assumptions and basic definitions

In this section we specify the physical assumptions on which our model is based.

1. The soil is a homogeneous, rigid porous medium.
2. The pollutant is adsorbed onto the soil grains. We neglect possible desorption.
3. The biomass is distributed in water as suspension (*free* biomass) or attached to the soil grains (*attached* biomass). In particular we neglect clusters formation in free biomass.
4. We neglect the bulk variation of density due to the free biomass (the density of bacteria is very close to the density of the water).
5. We consider the attachment of floating bacteria to the soil grains, but we neglect the inverse process.
6. The attached biomass forms another *porous medium*, supposed saturated at all times. The biofilm porosity is a known constant denoted by ε_b. Therefore, the attached biomass phase is considered as an incompressible mixture of solid biomass and immobile water having prescribed volume fractions. In the sequel we shall refer to the attached biomass also as *biomass gel*.
7. We focus on *anaerobic* processes only, i.e. we do not take into account consumption and diffusion of O_2 or other substances, considering the pollutant as the only nutrient.

We introduce the x coordinate for the 1-D spatial layer, $x \in [0, l]$, where $x = l$ represents the column top and $x = 0$ is the lower boundary. Moreover we specify the following notation:

- θ_{tot}, total moisture content: $\theta_{\text{tot}} = \theta + \theta_b$, where θ is the mobile-water content and θ_b is the water content in the biomass gel.
- ε_0, porosity of the biomass free medium.
- ϕ_s, solid matrix volume fraction: $\phi_s = 1 - \varepsilon_0$; ϕ_a, air volume fraction.
- ϕ_b, biomass gel volume fraction; $\varepsilon = \varepsilon_0 - \phi_b$ is the residual porosity.
  We thus have
  $$1 = \phi_s + \varepsilon_0 = \phi_s + \phi_a + \theta + \phi_b,$$
  so that the saturation condition is $\phi_a = 0$, namely
  $$\theta = \varepsilon = \varepsilon_0 - \phi_b.$$
- p_w, water pressure; p_a, air pressure (we set $p_a = 0$).
- Capillary pressure: $p_c = p_a - p_w = -p_w$.
- Pressure head (an admissible quantity since we are assuming no density variation): $\psi = -p_w/\varrho g = p_c/\varrho g$, $[\psi] = [L]$, where ϱ is the density of the liquid and

the free biomass. The model allows for $\psi = \psi(\theta, \phi_b)$, the dependence on ϕ_b being caused by the corresponding porosity reduction. The function $\psi = \psi(\theta, \phi_b)$ will be chosen later.

- Saturated permeability: k_{sat}, $[k_{\text{sat}}] = [L^2]$; relative permeability: $k_{\text{rel}} = k_{\text{rel}}(\theta, \phi_b)$, $[k_{\text{rel}}] = [-]$.
- Hydraulic conductivity: $K = \varrho g(k_{\text{sat}} k_{\text{rel}})/\mu$, $[K] = [LT^{-1}]$, where μ is the viscosity of the suspension, while k_{sat} and k_{rel} will be defined later.
- c, mass of adsorbed pollutant per unit mass of solid $[c] = [-]$.
- b, concentration of biomass in water $[b] = [ML^{-3}]$.

Using this notation the well-known Richards' equation describing the mass balance in the water flow trough the soil is

$$\frac{\partial}{\partial t}(\theta + \phi_b) + \frac{\partial}{\partial x} q(x,t) = 0,$$

where q is the *specific discharge* given by Darcy's law,

$$q = -K(\theta, b, \phi_b)\Big(\frac{\partial}{\partial x}\psi(\theta, \phi_b) + 1\Big),$$

whith a variable hydraulic conductivity function (see [8], for instance)

$$K(\theta, b, \phi_b) = \varrho g \frac{k_{\text{sat}}(\phi_b)}{\mu(b)} k_{\text{rel}}(\theta, \phi_b), \tag{2.1}$$

where for the viscosity μ we take a linear approximation

$$\mu = \mu(b) = \mu_0 + h_1 b, \tag{2.2}$$

with $h_1 > 0$ constant and where $\mu_0 = \mu(0)$ is the viscosity in the case of no biomass. We take a linear form also for k_{sat}:

$$k_{\text{sat}}(\phi_b) = k_{\text{sat}}^{(0)}\Big(1 - s_0 \frac{\phi_b}{\varepsilon_0}\Big), \tag{2.3}$$

where $0 < s_0 < 1$ is a constant and $k_{\text{sat}}^{(0)}$ is the saturation permeability value in the absence of biomass.

Concerning the selection of $\psi = \psi(\theta, \phi_b)$ and $k_{\text{rel}} = k_{\text{rel}}(\theta, \phi_b)$, we refer to Section 3.2.

In order to describe transport and evolution of the free biomass, we write down the usual advection/diffusion equation (see e.g. [9], [2]) completed by a growth and an attachment term, namely

$$\frac{\partial}{\partial t}[\theta b] = \underbrace{-\frac{\partial}{\partial x}[q(x,t)b] + \frac{\partial}{\partial x}\Big[D_b\theta\frac{\partial b}{\partial x}\Big]}_{\text{advection/diffusion}} + \underbrace{h_2[B_{\max}f(c) - b]\theta b}_{\text{free biomass growth}} - \underbrace{\lambda\theta b}_{\text{attachment}}, \tag{2.4}$$

where:

- For the sake of simplicity, we assume that the diffusion coefficient D_b is constant (while, in general, it should be specified as the sum of dispersion and molecular diffusion coefficients, which in turn depend on velocity and bacteria concentration, respectively). This corresponds to considering sufficiently slow flows.
- The biomass growth is modeled by a *logistic-type* dynamics, where the *carrying capacity* $B_{\max}$ is modulated by a function $f(c)$ ranging in $(0,1)$, to take into account also additional effects, like e.g. *toxicity* of the pollutant at high concentrations.
- λ is the attachment coefficient.

A similar argument is used to describe the growth of the attached biomass, that is,

$$\frac{\partial \phi_b}{\partial t} = \underbrace{h_2[\varepsilon_0 f(c) - \phi_b]\phi_b}_{\text{biomass growth}} + \underbrace{\lambda\theta b}_{\text{attachment}}. \tag{2.5}$$

Finally, the evolution of the pollutant is driven by the bio-reduction process, i.e.

$$\frac{\partial c}{\partial t} = -h_{BD}\phi_b c, \tag{2.6}$$

h_{BD} being the bioreduction specific rate.

2.2. The complete system of equations

The problem to be studied is the following system of PDEs (2.7)–(2.9) endowed with initial and boundary conditions (2.11)–(2.18)

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x}\Big[K(\theta, b, \phi_b)\Big(\frac{\partial}{\partial x}\psi(\theta,\phi_b) + 1\Big)\Big] - \frac{\partial \phi_b}{\partial t}, \tag{2.7}$$

$$\frac{\partial}{\partial t}(\theta b) = -\frac{\partial}{\partial x}(qb) + D_b\frac{\partial}{\partial x}\Big(\theta\frac{\partial b}{\partial x}\Big) + h_2[B_{\max}f(c) - b]\theta b - \lambda\theta b, \tag{2.8}$$

$$\frac{\partial \phi_b}{\partial t} = h_2[\varepsilon_0 f(c) - \phi_b]\phi_b + \lambda\theta b, \tag{2.9}$$

$$\frac{\partial c}{\partial t} = -h_{BD}\phi_b c, \tag{2.10}$$

$$\theta(x,0) = \Theta_0(x), \tag{2.11}$$

$$b(x,0) = b_0, \tag{2.12}$$

$$c(x,0) = c_0, \tag{2.13}$$

$$\phi_b(x,0) = 0, \tag{2.14}$$

$$\theta(l,t) = \Theta_l(t), \tag{2.15}$$

$$b(l,t) = b_0, \tag{2.16}$$

$$\theta(0,t) = \varepsilon(t), \tag{2.17}$$

$$\frac{\partial b}{\partial x}(0,t) = 0. \tag{2.18}$$

For simplicity of exposition we take b_0 and c_0 constant (and positive), but this assumption can be somewhat relaxed. The Dirichlet data (2.15), (2.16) could be replaced by conditions of different type.

3. Existence for the complete system, locally in time

In this section we shall prove the existence of a set (θ, c, b, ϕ_b) solving the system of PDEs in a sufficiently small time interval.

3.1. Notation

Here we list the symbols denoting spaces and norms used in the paper.

Considering $\Omega \subset \mathbb{R}$, $T > 0$ and $\Omega_T = \Omega \times (0,T)$, as usual we denote by $C^{m,n}(\Omega_T)$ the set of all continuous functions whose m space derivatives in x and n time derivatives in t are continuous in Ω_T. When $m = 0 = n$ we denote by $C(\Omega_T)$ the set of continuous functions in Ω_T, whose norm is

$$\|u\|_0 = \sup_{(x,t)\in\Omega_T} |u(x,t)|.$$

When a function $u \in C(\Omega_T)$ is Hölder continuous of order $\nu \in (0,1)$, we denote the Hölder constant as

$$\langle u \rangle_\nu = \sup\Big\{ \frac{|u(x,t) - u(\xi,\tau)|}{(|t-\tau| + |x-\xi|^2)^{\nu/2}},\ \forall\,(x,t),(\xi,\tau) \in \Omega_T \Big\}$$

and the Hölder norm of u is

$$\|u\|_\nu = \|u\|_0 + \langle u \rangle_\nu\,.$$

The set of Hölder continuous functions in Ω_T with finite Hölder norm is denoted by $C^\nu(\Omega_T)$. Similarly, the sets of functions in $C^\nu(\Omega_T)$ with finite norms

$$\|u\|_{1+\nu} = \|u\|_0 + \langle u_x \rangle_\nu + \langle u_t \rangle_\nu \,,$$
$$\|u\|_{2+\nu} = \|u\|_0 + \langle u_x \rangle_\nu + \langle u_{xx} \rangle_\nu + \langle u_t \rangle_\nu \,,$$

are denoted by $C^{1+\nu}$ and $C^{2+\nu}$, respectively.

3.2. Assumptions

We stipulate the following assumptions.

(H.1) The function $\psi(\theta, \phi_b)$ is defined for instance in the following way: for any $\phi_b \in \mathbb{R}$,

$$\psi(\theta, \phi_b) = \begin{cases} \psi_r\Big(1 - \dfrac{\theta}{\varepsilon_0 - \phi_b}\Big), & \text{for } \theta < \varepsilon_0 - \phi_b, \\ \in [0, +\infty), & \text{for } \theta = \varepsilon_0 - \phi_b, \end{cases} \tag{3.1}$$

where $\psi_r < 0$ is a constant (once more, linearity is assumed for simplicity). For $\theta < \varepsilon_0 - \phi_b$ we can have any smooth function such that both $\partial\psi/\partial\theta$ and $\partial\psi/\partial\phi_b$ are positive.

(H.2) For any $\phi_b \in \mathbb{R}$, $k_{\mathrm{rel}}(\theta, \phi_b)$ is a smooth increasing and non-negative function w.r.t. θ for $\theta \in [0, \varepsilon_0 - \phi_b]$, while $k_{\mathrm{rel}}(\theta, \phi) \equiv 1$ for $\theta \in [\varepsilon_0 - \phi_b, +\infty)$. For instance (see also [5]),

$$k_{\mathrm{rel}}(\theta, \phi_b) = \Big(\frac{\theta}{\varepsilon(\phi_b)}\Big)^3 = \Big(\frac{\theta}{\varepsilon_0 - \phi_b}\Big)^3. \tag{3.2}$$

Moreover, for a given constant $\delta \in (0, \varepsilon_0)$ we define

$$G(\delta) = \sup_{\substack{\phi_b \in (0, \varepsilon_0 - \delta) \\ \theta \in (0, \varepsilon_0 - \phi_b)}} \Big| \frac{\partial k_{\mathrm{rel}}}{\partial \theta}(\theta, \phi_b) \Big|. \tag{3.3}$$

(H.3) Concerning the function $f = f(c)$, let m and m_1 be two constants, $0 < m < 1$, $m_1 > 1$, and assume that

- $f\colon\ [0, +\infty) \to [0, 1]$, $f(z) \in C^\infty$;
- *proliferation range*[1]: $\forall\, z \in [0, mc_0]$, $0 \leqslant f(z) \leqslant 1$, and f is monotone increasing with $f'(mc_0) = 0$;

[1] For simplicity we set here the optimal proliferation threshold (mc_0) and the toxicity threshold ($m_1 c_0$) in dependence on the initial value c_0. A more general definiton of these parameters can be given, see [2] and the references therein.

- *"optimal" proliferation range*; $\forall\, z \in (mc_0, m_1c_0]$, $f(z) \equiv 1$;
- *toxicity range*: $\forall\, z > m_1c_0$, $0 \leqslant f(z) \leqslant 1$, and f is monotone decreasing. In particular, we define

$$\Gamma_1 = \max_{z\in\mathbb{R}} f'(z), \tag{3.4}$$

$$\Gamma_2 = \max_{z\in\mathbb{R}} |f''(z)|. \tag{3.5}$$

(H.4) The given initial condition $\Theta_0(x)$ satisfies $\Theta_0(x) \in C^{2+\alpha}([0,l])$ for a given $\alpha \in (0,1)$ and $0 < \Theta_{\min} \leqslant \Theta_0(x) \leqslant \varepsilon_0 - \delta$, for all $x \in [0,l]$ and some $\delta \in (0,\varepsilon_0)$.
Moreover, in (2.12), (2.13) and (2.16) we assume

$$0 < b_0 \leqslant B_{\max} f(c_0) \quad \text{and} \quad c_0 > 0.$$

Concerning $\Theta_l(t)$ we require $\Theta_l \in C^{1+\alpha}([0,T])$ and $0 < \Gamma_3 \leqslant \Theta_l(t) \leqslant \varepsilon_0 - \phi_b(l,t) - \delta$, for all $t \in [0,T]$.
Finally, we assume the compatibility condition:

$$\Theta_0(l) = \Theta_l(0).$$

Moreover, for each time $T > 0$ we define $\phi_{\max} = \phi_{\max}(T)$ as

$$\phi_{\max}(T) = \frac{\lambda B_{\max}}{h_2} \exp(h_2 T), \tag{3.6}$$

which satisfies $\phi_{\max}(T) < (\varepsilon_0 - \delta)$ for T such that

$$T < T_{\max} = \frac{1}{h_2(\varepsilon_0 - \delta)} \log\Big(\frac{h_2(\varepsilon_0 - \delta)}{\lambda B_{\max}}\Big). \tag{3.7}$$

Finally, for $T \in [0, (\varepsilon_0 - \delta - \Gamma_3)/\Phi]$, $\Phi = \varepsilon_0(h_2\phi_{\max} + \lambda B_{\max})$ and $\alpha \in (0,1)$, we introduce the following function spaces

$$V_1(R_1) = \Big\{\phi_b \in C^{2+\alpha}(D_T)\colon\ 0 \leqslant \phi_b(x,t) \leqslant \phi_{\max},\ 0 \leqslant \frac{\partial \phi_b}{\partial t}(x,t) \leqslant \Phi, \quad \|\phi_b\|_{2+\alpha} \leqslant R_1\Big\}, \tag{3.8}$$

$$V_2(R_2, \overline{R}_2) = \{b \in C^{2+\alpha}(D_T)\colon\ 0 \leqslant b(x,t) \leqslant B_{\max},\ \|b\|_{1+\alpha} \leqslant \overline{R}_2, \quad \|b\|_{2+\alpha} \leqslant R_2\}, \tag{3.9}$$

$$V_3(R_3, \overline{R}_3) = \{\theta \in C^{2+\alpha}(D_T)\colon\ 0 < \Gamma_3 \leqslant \theta(x,t) \leqslant \varepsilon_0 - \delta - \Phi t, \quad \theta(x,0) = \Theta_0(x),\ \|\theta\|_{1+\alpha} \leqslant \overline{R}_3,\ \|\theta\|_{2+\alpha} \leqslant R_3\}, \tag{3.10}$$

where $\Gamma_3 < \Theta_{\min}$ and R_1, R_2, $\overline{R}_2$, R_3 and $\overline{R}_3$ are constants to be specified later on. Note that the definition of V_3 is consistent with the non-saturation assumption.

The selection of the norms in the sets V_1, V_2, V_3 is such that all the uniform estimates that will be derived in the next section refer to the stronger norm $C^{2+\alpha}$, fixed by the data, while a weaker norm $C^{2+\nu}$, $0 < \nu < \alpha$, will be used to show the continuity of the various mappings that will be introduced. In this way we plan to use Schauder's fixed point theorem in the topology $C^{2+\nu}$, with the higher norm $C^{2+\alpha}$ providing compactness.

3.3. Existence of a mapping from $V_1 \times V_2$ into itself

We proceed in several steps.

Proposition 3.1. *If assumptions* (H.1)–(H.4) *are fulfilled, then for any triple* $(\phi_b, b, \theta) \in V_1 \times V_2 \times V_3$, *there exists a unique function* $c \in C^{2+\alpha}(D_T)$ *solving the Cauchy problem* (2.10), (2.13), *i.e.*

$$\begin{aligned} \frac{\partial c}{\partial t} &= -h_{BD}\phi_b c, \\ c(x,0) &= c_0. \end{aligned}$$

Further, once $c(x,t)$ *is determined, there exists a unique function* $\varphi \in C^{2+\alpha}(D_T)$ *solving the following Cauchy problem*

$$\begin{cases} \dfrac{\partial \varphi}{\partial t} = h_2[\varepsilon_0 f(c) - \phi_b]\varphi + \lambda\theta b, \\ \varphi(x,0) = 0. \end{cases} \tag{3.11}$$

Moreover, for T *satisying* (3.7) *we have*

$$0 \leqslant c(x,t) \leqslant c_0, \tag{3.12}$$

$$0 \leqslant \varphi(x,t) \leqslant \phi_{\max} < \varepsilon_0, \tag{3.13}$$

$$0 \leqslant \frac{\partial \varphi}{\partial t} \leqslant \Phi, \tag{3.14}$$

and the following estimates hold true

$$\|c - c_0\|_{2+\alpha} \leqslant p_1 T \|\phi_b\|_{2+\alpha}, \tag{3.15}$$

$$\|\varphi\|_{2+\alpha} \leqslant p_2 T(\|\phi_b\|_{2+\alpha} + \|b\|_{2+\alpha} + \|\theta\|_{2+\alpha}), \tag{3.16}$$

where p_1 *and* p_2 *are positive constants such that*

$$\begin{aligned} p_1 &= p_1(c_0, h_{BD}, \varepsilon_0, h_2, \lambda), \\ p_2 &= p_2(c_0, h_{BD}, \varrho_b, \varepsilon_0, h_2, \lambda, \Gamma_1, \Gamma_2, \Gamma_3). \end{aligned}$$

P r o o f. Once $(\phi_b, b, \theta) \in V_1 \times V_2 \times V_3$ are given, in a straightforward way we are able to write down the explicit solution to the problem (2.10), (2.13), namely

$$c(x,t) = c_0 \exp\left[-h_{BD} \int_0^t \phi_b(x,\tau)\,\mathrm{d}\tau\right], \tag{3.17}$$

from which $\partial c/\partial x$ and $\partial^2 c/\partial x^2$ can be calculated explicitly in order to obtain the estimate (3.15). Also the property (3.12) is obtained directly from the expression (3.17).

On the other hand, once $c(x,t)$ is obtained, we can write also the explicit solution to the problem (3.11), i.e.

$$\varphi(x,t) = \lambda \int_0^t \theta(x,\tau) b(x,\tau) \exp\left[h_2 \int_\tau^t (\varepsilon_0 f(c(x,\eta)) - \phi_b(x,\eta))\,\mathrm{d}\eta\right] \mathrm{d}\tau. \tag{3.18}$$

From (3.18) we can get the expressions for $\partial\varphi/\partial x$ and $\partial^2\varphi/\partial x^2$, eventually deriving the estimate (3.16).

Moreover, recalling that $\phi_b \in V_1$ and the assumption (H.3), we have

$$\varepsilon_0 f(c) - \phi_b \leqslant \varepsilon_0 - \phi_b \leqslant \varepsilon_0,$$

so that, because of $(b,\theta) \in V_2 \times V_3$ and (3.6), from (3.18) we get

$$\begin{aligned} 0 \leqslant \varphi(x,t) &\leqslant \lambda\varepsilon_0 B_{\max} \int_0^t \exp[h_2(t-\tau)]\,\mathrm{d}\tau = \frac{\lambda B_{\max}}{h_2}[\exp(h_2\varepsilon_0 t) - 1] \\ &\leqslant \frac{\lambda B_{\max}}{h_2} \exp(h_2\varepsilon_0 T_{\max}) = \phi_{\max} < \varepsilon_0, \end{aligned}$$

so that the property (3.13) is satisfied.

Finally, let us prove (3.14). The upper bound Φ is easily found directly from the expression (3.11). Concerning the lower bound, we know that $\varphi(t=0) = 0$ and $\partial\varphi/\partial t(t=0) = \lambda\theta(t=0)b_0 > 0$. Let $t^* > 0$ be the first time in $(0,T]$ such that $\partial\varphi/\partial t(t=t^*) = 0$. It follows that for $t \in (0,t^*]$, $\varphi > 0$ and, from (3.11),

$$[\varepsilon_0 f(c) - \phi_b]\varphi(t=t^*) + \lambda\theta b = 0 \Rightarrow [\varepsilon_0 f(c) - \phi_b] \leqslant 0.$$

Denoting $c^* = c(t=t^*)$, we then have

$$f(c^*) \leqslant \frac{\phi_b}{\varepsilon_0} \leqslant \frac{\phi_{\max}}{\varepsilon_0},$$

so that, exploiting the expression (3.17),

$$c^* \geqslant c_0 \exp[-h_{BD}\varepsilon_0 t^*],$$

we get

$$-h_{BD}\varepsilon_0 t^* \leqslant \log\Big[f^{-1}\Big(\frac{\phi_{\max}}{\varepsilon_0}\Big)\Big],$$

namely,

$$t^* \geqslant -\log\Big[f^{-1}\Big(\frac{\phi_{\max}}{\varepsilon_0}\Big)\Big]\frac{1}{h_{BD}\varepsilon_0}. \tag{3.19}$$

The estimate (3.19) is a lower bound for the time at which φ_t changes its sign. It means that if the time scale we are considering, $T < T_{\max}$, is less than or equal to the right-hand side of (3.19), we have

$$\frac{\partial\varphi}{\partial t} \geqslant 0 \quad \text{in } [0,T].$$

□

Corollary 3.1 (Continuous dependence for φ). *In the framework of Proposition* 3.1, *if we consider two triples* $(\phi_{b,1}, b_1, \theta_1), (\phi_{b,2}, b_2, \theta_2) \in V_1 \times V_2 \times V_3$ *and the corresponding* φ_1, φ_2, *then we have*

$$\|\varphi_1 - \varphi_2\|_{2+\nu} \leqslant r_1 T(\|\phi_{b,1} - \phi_{b,2}\|_{2+\nu} + \|b_1 - b_2\|_{2+\nu} + \|\theta_1 - \theta_2\|_{2+\nu}) \tag{3.20}$$

where r_1 *is a positive constant such that*

$$r_1 = p_3(c_0, h_{BD}, \varepsilon_0, h_2, \lambda, \Gamma_1, \Gamma_2, \Gamma_3, \delta).$$

To get the desired estimate it is sufficient to write the explict expression for $(\varphi_1 - \varphi_2)$ and its derivatives, starting from (3.18). □

Proposition 3.2. *If the assumptions* (H.1)–(H.4) *are fulfilled and* T *is sufficiently small (see* (3.7) *and* (3.29)*), then for any triple* $(\phi_b, b, \theta) \in V_1 \times V_2 \times V_3$ *there exists a unique function* $\beta \in C^{2+\alpha}(D_T)$ *solving the following problem*

$$\theta\frac{\partial\beta}{\partial t} = D_b\frac{\partial}{\partial x}\Big(\theta\frac{\partial\beta}{\partial x}\Big) - \frac{\partial}{\partial x}(q\beta) + \Big\{h_2[B_{\max}f(c) - \beta]\theta - \lambda\theta - \frac{\partial\theta}{\partial t}\Big\}\beta, \tag{3.21}$$

$$\beta(x,0) = b_0, \tag{3.22}$$

$$\beta(l,t) = b_0, \tag{3.23}$$

$$\frac{\partial\beta}{\partial x}(0,t) = 0, \tag{3.24}$$

where

$$q = q(x,t) = -K(\theta, b, \phi_b)\Big(\frac{\partial}{\partial x}\psi(\theta,\phi_b) + 1\Big).$$

Moreover, we have

$$0 \leqslant \beta(x,t) \leqslant B_{\max}, \tag{3.25}$$

and

$$\|\beta\|_{2+\alpha} \leqslant p_4(\|\phi_b\|_{2+\alpha} + \|\theta\|_{2+\alpha} + \|b\|_{1+\alpha}), \tag{3.26}$$

where p_4 is a positive constant such that

$$p_4 = p_4\big(\varrho, g, k_{\rm sat}^{(0)}, \mu_0, \mu_1, \psi_r, G_1(\phi_{\max}), \phi_{\max}, \varepsilon_0, \delta, \alpha, \lambda, h_2, B_{\max}, \Gamma_3, D_b, T_{\max}\big).$$

P r o o f. Let us examine the coefficients in the equation (3.21), which we rewrite in the following way

$$\frac{\partial\beta}{\partial t} = D_b\frac{\partial^2\beta}{\partial x^2} + \frac{1}{\theta}\Big(D_b\frac{\partial\theta}{\partial x} - q\Big)\frac{\partial\beta}{\partial x} + \Big\{h_2[B_{\max}f(c) - \beta] - \lambda - \frac{1}{\theta}\Big(\frac{\partial\theta}{\partial t} + \frac{\partial q}{\partial x}\Big)\Big\}\beta. \tag{3.27}$$

Since $\theta \in V_3$, we have to check only the boundness of q and its first spatial derivative. More precisely, we have

$$|q| \leqslant |K(\theta, b, \phi_b)|\Big(\Big|\frac{\partial\psi}{\partial\theta}\Big|\Big|\frac{\partial\theta}{\partial x}\Big| + \Big|\frac{\partial\psi}{\partial\phi}\Big|\Big|\frac{\partial\phi}{\partial x}\Big| + 1\Big).$$

Moreover, by the assumtpions (H.1)–(H.2), we get

$$\frac{|\psi_r|}{\varepsilon_0} \leqslant \frac{\partial\psi}{\partial\theta} \leqslant \frac{|\psi_r|}{\varepsilon_0 - \phi_{\max}} \quad \text{and} \quad \frac{|\psi_r|\Gamma_3}{\varepsilon_0^2} \leqslant \frac{\partial\psi}{\partial\phi_b} \leqslant \frac{|\psi_r|\varepsilon_0}{(\varepsilon_0 - \phi_{\max})^2},$$

so that

$$|q| \leqslant \varrho g\frac{k_{\rm sat}^{(0)}}{\mu_0}\Big\{\Big|\frac{\partial\theta}{\partial x}\Big|\Big|\frac{\psi_r}{\varepsilon_0 - \phi_{\max}}\Big| + \Big|\frac{\partial\phi_b}{\partial x}\Big|\frac{|\psi_r|\varepsilon_0}{(\varepsilon_0 - \phi_{\max})^2} + 1\Big\}.$$

Further, we exploit again the assumptions (H.1)–(H.2) to get the following estimates

$$\Big|\frac{\partial K}{\partial\theta}\Big| \leqslant \varrho g\frac{k_{\rm sat}^{(0)}}{\mu_0}G_1(\phi_{\max}),$$

$$\Big|\frac{\partial K}{\partial b}\Big| \leqslant \mu_1\varrho g\frac{k_{\rm sat}^{(0)}}{\mu_0^2},$$

$$\Big|\frac{\partial K}{\partial\phi_b}\Big| \leqslant \frac{3\varepsilon_0^3}{(\varepsilon_0 - \phi_{\max})^2},$$

$$\Big|\frac{\partial^2}{\partial x^2}\psi(\theta,\phi_b)\Big| \leqslant |\psi_r|\Big\{\frac{1}{(\varepsilon_0 - \phi_{\max})^2}\Big[2\Big|\frac{\partial\phi_b}{\partial x}\Big|\Big|\frac{\partial\theta}{\partial x}\Big| + \Big|\frac{\partial^2\phi_b}{\partial x^2}\Big||\theta|\Big] + \frac{1}{\varepsilon_0 - \phi_b}\Big|\frac{\partial^2\theta}{\partial x^2}\Big| + \frac{2|\theta|}{|(\varepsilon_0 - \phi_b)^3|}\Big|\frac{\partial\phi_b}{\partial x}\Big|\Big\}.$$

Therefore, we get

$$\left|\frac{\partial q}{\partial x}(x,t)\right| \leqslant C$$

where C is a constant depending on ψ_r, ε_0, δ, α, $\phi_{\max}$, ϱ, g, $k_{\mathrm{sat}}^{(0)}$, μ_0, μ_1, $G_1(\phi_{\max})$ and R_1, $\overline{R}_2$ and R_3.

Now, we are in position to apply Theorem 5.2, Ch. VI, p. 564 and Remark 5.1 of [4], so that the existence of a unique solution $\beta \in C^{2+\alpha}(D_T)$ is obtained. Moreover, the same reference gives the desired estimate (3.26).

As to (3.25), we note that $\bar{u} \equiv 0$ is a lower solution for the problem for β, so that

$$\beta(x,t) \geqslant 0, \quad \forall\,(x,t) \in D_T.$$

On the other hand, once the existence of a solution is proved, one can reformulate the problem for (3.27) as a linear problem and rewrite it in a compact form, i.e.

$$\begin{cases} v_t - \mathcal{L}(v) = -h_2\beta^2(x,t) + F(x,t)v, \\ v(x,0) = b_0, \\ v(l,t) = b_0, \\ v_x(0,t) = 0, \end{cases} \tag{3.28}$$

where $\mathcal{L}$ denotes the elliptic operator in (3.27) and

$$F(x,t) = \left\{h_2 B_{\max} f(c) - D_b\frac{\partial q}{\partial x} - \lambda - \frac{1}{\theta}\frac{\partial\theta}{\partial t}\right\}.$$

We have

$$F(x,t) \leqslant h_2 B_{\max} + D_b C + \frac{1}{\Gamma_3}\|\theta\|_{2+\alpha} =: \gamma_1 > 0.$$

As usual, we take some $\gamma > 0$ such that $\gamma \geqslant \gamma_1$ and define

$$u(x,t) = \mathrm{e}^{-\gamma t}v(x,t).$$

It is easily seen from (3.28) that u satisfies

$$\begin{cases} u_t - \mathcal{L}(u) + (\gamma - F(x,t))u = -h_2\beta^2\mathrm{e}^{-\gamma t} \leqslant 0, \\ u(x,0) = b_0, \\ u(l,t) = \mathrm{e}^{-\gamma t}b_0, \\ \dfrac{\partial u}{\partial x}(0,t) = 0, \end{cases}$$

with $(\gamma - F(x,t)) \geqslant 0$. Thus, the maximum principle for parabolic operators entails

$$u(x,t) \leqslant b_0,$$

namely,

$$v(x,t) \leqslant \mathrm{e}^{\gamma t} b_0.$$

Therefore, if

$$T \leqslant \frac{1}{\gamma} \log\Big(\frac{B_{\max}}{b_0}\Big), \tag{3.29}$$

we have the desired upper bound in (3.25). □

In the following proposition we introduce an additional estimate for $\|\beta\|_{1+\alpha}$ which will be used to prove Theorem 3.1 below.

Proposition 3.3. *The function $\beta \in C^{2+\alpha}(D_T)$ found in Proposition 3.2 satisfies the following estimate*

$$\|\beta - b_0\|_{1+\alpha} \leqslant T^{\gamma}\{p_5' \|b\|_{1+\alpha} + p_5(\|\phi_b\|_{2+\alpha} + \|\theta\|_{2+\alpha})\}, \tag{3.30}$$

with some constants p_5 and p_5' depending on the same quantities as p_4, where the exponent γ depends in particular on α.

P r o o f. From the estimate (3.23), p. 200 of [3], immediately applicable to $\beta - b_0$, it follows that the norm $\|\beta - b_0\|_{1+\alpha}$ is dominated by the sup-norm of the free term in (3.21) multiplied by a factor tending to zero as $T \to 0$ like some power T^{γ}. □

Proposition 3.4 (Continuous dependence for β)**.** *In the framework of Proposition (3.2), if we consider two triples $(\phi_{b,1}, b_1, \theta_1), (\phi_{b,2}, b_2, \theta_2) \in V_1 \times V_2 \times V_3$ and the corresponding β_1, β_2, then we have*

$$\|\beta_1 - \beta_2\|_{2+\nu} \leqslant r_4(\|\phi_{b,1} - \phi_{b,2}\|_{2+\nu} + \|b_1 - b_2\|_{2+\nu} + \|\theta_1 - \theta_2\|_{2+\nu}) \tag{3.31}$$

where r_4 is a positive constant such that

$$r_4 = r_4\big(D_b, h_2, B_{\max}, \phi_{\max}, c_0, \varepsilon_0, \lambda, \varrho, g, k_{\text{sat}}^{(0)}, \mu_0, \psi_r, \delta\big).$$

P r o o f. Let us define $w(x,t) = (\beta_1(x,t) - \beta_2(x,t))$. Then w satisfies the following problem

$$\frac{\partial w}{\partial t} = D_b \frac{\partial^2 w}{\partial x^2} + A(x,t)\frac{\partial w}{\partial x} + B(x,t)w + C(x,t), \tag{3.32}$$

$$w(x,0) = 0, \tag{3.33}$$

$$w(l,t) = 0, \tag{3.34}$$

$$\frac{\partial w}{\partial x}(0,t) = 0, \tag{3.35}$$

where

$$A(x,t) = \frac{1}{\theta_1}\Big[D_b \frac{\partial \theta_1}{\partial x} - q_1\Big],$$

$$B(x,t) = h_2[B_{\max} f(c_1) - \beta_1] - \lambda - \frac{1}{\theta_1}\Big(\frac{\partial \theta_1}{\partial t} + \frac{\partial q_1}{\partial x}\Big) - h_2\beta_2,$$

$$C(x,t) = \Big\{\frac{1}{\theta_1}\Big(D_b \frac{\partial \theta_1}{\partial x} - q_1\Big) - \frac{1}{\theta_2}\Big(D_b \frac{\partial \theta_2}{\partial x} - q_2\Big)\Big\}\frac{\partial \beta_2}{\partial x}$$
$$+ \beta_2\Big\{h_2 B_{\max}(f(c_1) - f(c_2)) - \frac{1}{\theta_1}\Big(\frac{\partial \theta_1}{\partial t} + \frac{\partial q_1}{\partial x}\Big) + \frac{1}{\theta_2}\Big(\frac{\partial \theta_2}{\partial t} + \frac{\partial q_2}{\partial x}\Big)\Big\}.$$

In particular, recalling (3.26), we can easily obtain the following estimate for the free term $C(x,t)$,

$$\|C\|_\nu \leqslant r_2(\|b_1 - b_2\|_{2+\nu} + \|\theta_1 - \theta_2\|_{2+\nu} + \|\phi_{b,1} - \phi_{b,2}\|_{2+\nu}), \tag{3.36}$$

where

$$r_2 = r_2\big(D_b, h_2, B_{\max}, \phi_{\max}, c_0, \varepsilon_0, \delta, \alpha, \lambda, \varrho, g, k_{\mathrm{sat}}^{(0)}, \mu_0.\mu_1, \psi_r, G_1(\phi_{\max})\big).$$

Therefore, to the linear problem (3.32)–(3.35) we apply Theorem 5.2, p. 320 of [4], stating the existence of a unique solution $w \in C^{2+\nu}(D_T)$ for which the following estimate holds true

$$\|w\|_{2+\nu} \leqslant r_3\|C\|_\nu, \tag{3.37}$$

where r_3 is a constant not depending on $C(x,t)$. Thus, (3.36) and (3.37) entail

$$\|\beta_1 - \beta_2\|_{2+\nu} \leqslant r_4(\|b_1 - b_2\|_{2+\nu} + \|\theta_1 - \theta_2\|_{2+\nu} + \|\phi_{b,1} - \phi_{b,2}\|_{2+\nu}),$$

and the proof is complete. □

Theorem 3.1. *Let us consider $\theta \in V_3$. If the assumptions* (H.1)–(H.4) *are fulfilled, then for a sufficiently small T, there is a solution $(\phi_b, b, c) \in [C^{2+\alpha}(D_T)]^3$ to the following system*

$$\frac{\partial}{\partial t}(\theta b) = -\frac{\partial}{\partial x}(qb) + D_b \frac{\partial}{\partial x}\Big(\theta \frac{\partial b}{\partial x}\Big) + h_2[B_{\max} f(c) - b]\theta b - \lambda\theta b, \tag{3.38}$$

$$\frac{\partial \phi_b}{\partial t} = h_2[\varepsilon_0 f(c) - \phi_b]\phi_b + \lambda\theta b, \tag{3.39}$$

$$\frac{\partial c}{\partial t} = -h_{BD}\phi_b c, \tag{3.40}$$

$$b(x,0) = b_0, \tag{3.41}$$

$$c(x,0) = c_0, \tag{3.42}$$

$$b(l,t) = b_0, \tag{3.43}$$

$$\frac{\partial b}{\partial x}(0,t) = 0. \tag{3.44}$$

P r o o f. For any $\theta \in V_3$, we define on the space $V_1 \times V_2$ the mapping Λ_θ by

$$\Lambda_\theta(\phi_b, b) = (\varphi, \beta),$$

where (φ, β) are the functions given by Propositions 3.2 and 3.4. If we prove that

1. Λ_θ is continuous in the topology $C^{2+\nu}$,
2. $\Lambda_\theta(V_1 \times V_2) \subset V_1 \times V_2$,

then, since $V_1 \times V_2$ is compact,[2] it follows that Λ_θ is a completely continuous mapping. Therefore, Schauder's theorem can be applied to show the existence of a fixed point. The latter is a solution (ϕ_b, b) to the problem (3.38)–(3.44).

The assertion 1 is a straightforward consequence of Corollary 3.1 and Proposition 3.4.

To prove the assertion 2, we have to choose a suitable T and impose some constraint on the constants R_1, R_2, $\overline{R}_2$ and R_3 introduced in (3.8)–(3.10). From (3.30) we see that our first requirement is

$$\overline{R}_2 \geqslant T^\gamma \{p_5' \, \overline{R}_2 + p_5(R_1 + R_2)\},$$

which for T suitably small allows to choose

$$\overline{R}_2 = \frac{T^\gamma p_5}{1 - p_5' \, T^\gamma}(R_1 + R_3). \tag{3.45}$$

Next, using (3.16) and (3.26) we impose

$$\|\phi\|_{2+\alpha} \leqslant p_2 T(R_1 + R_2 + R_3),$$
$$\|\beta\|_{2+\alpha} \leqslant p_4(\overline{R}_2 + R_1 + R_3),$$

leading to the conditions

$$R_1 \geqslant p_2 T(R_1 + R_2 + R_3),$$
$$R_2 \geqslant p_4'(R_1 + R_2),$$

[2] Indeed, the topology of the spaces V_i to be used to test the continuity of the mapping is the one induced by $\| \cdot \|_{2+\nu}$. However, the sets V_i are uniformly bounded in $C^{2+\alpha}$, $\alpha > \nu$, so that they are compact sets in $C^{2+\nu}$.

with $p'_4 = p_4[1 + T^\gamma p_5/(1 - p'_5 T^\gamma)]$, which we rewrite in the form

$$R_1 \geqslant \frac{p_2 T}{1 - p_2 T}(R_2 + R_3), \tag{3.46}$$

$$R_1 \leqslant \frac{R_2}{p'_4} - R_3. \tag{3.47}$$

For all $R_3 > 0$ and all compatible T (i.e. T less than some T^* depending on p_2, p_4, p_5, p'_5) the above inequalities define an admissible region $\mathcal{R}$ in the quarter plane $R_1 > 0$, $R_2 > 0$.

Therefore, for a given R_3, taking $(R_1, R_2) \in \mathcal{R}$ we have

$$\Lambda_\theta(V_1 \times V_2) \subset V_1 \times V_2,$$

and the proof is complete. □

3.4. Existence of a mapping from V_3 into itself

Throughout this section we denote by p_i, $i = 6, 7, \ldots$, constants depending on the same parameters as p_4.

The next step is to consider Richards' equation (2.7) which we rewrite in the following way,

$$\begin{aligned}\frac{\partial\theta}{\partial t} = {} & \Big[K(\theta, b, \phi_b)\frac{\partial\psi}{\partial\theta}\Big]\frac{\partial^2\theta}{\partial x^2} + \Big[\Big(\frac{\partial K}{\partial\theta}\frac{\partial\theta}{\partial x} + \frac{\partial K}{\partial\phi_b}\frac{\partial\phi_b}{\partial x} + \frac{\partial K}{\partial b}\frac{\partial b}{\partial x}\Big)\frac{\partial\psi}{\partial\theta} \\ & + \Big(\frac{\partial K}{\partial\theta}\frac{\partial\psi}{\partial\phi_b}\frac{\partial\phi_b}{\partial x}\Big) + K(\theta, b, \phi_b)\frac{\partial}{\partial x}\Big(\frac{\partial\psi}{\partial\theta}\Big) + \frac{\partial K}{\partial\theta} + K(\theta, b, \phi_b)\frac{\partial^2\psi}{\partial\phi_b\partial\theta}\frac{\partial\phi_b}{\partial x}\Big]\frac{\partial\theta}{\partial x} \\ & + \Big[K(\theta, b, \phi_b)\Big(\frac{\partial^2\psi}{\partial\phi_b^2}\Big(\frac{\partial\phi_b}{\partial x}\Big)^2 + \frac{\partial\psi}{\partial\phi_b}\frac{\partial^2\phi_b}{\partial x^2}\Big) \\ & + \Big(\frac{\partial K}{\partial b}\frac{\partial b}{\partial x} + \frac{\partial K}{\partial\phi_b}\frac{\partial\phi_b}{\partial x}\Big)\Big(1 + \frac{\partial\psi}{\partial\phi_b}\frac{\partial\phi_b}{\partial x}\Big) - \frac{\partial\phi_b}{\partial t}\Big].\end{aligned}$$

Now we take some $\theta \in V_3$ and the pair (ϕ_b, b) as the corresponding fixed point $(\phi_b, b) = \Lambda_\theta(\phi_b, b)$ and we write the linear system

$$\frac{\partial z}{\partial t} = \mathcal{A}(x,t)\frac{\partial^2 z}{\partial x^2} + \mathcal{B}(x,t)\frac{\partial z}{\partial x} - (\lambda b)z + \mathcal{C}(x,t), \tag{3.48}$$

$$z(x, 0) = \Theta_0(x), \tag{3.49}$$

$$z(0, t) = \varepsilon(0, t) = \varepsilon_0 - \phi_b(0, t), \tag{3.50}$$

$$z(l, t) = \Theta_l(t), \tag{3.51}$$

where

$$\mathcal{A}(x,t) = \Big[K(\theta,b,\phi_b)\frac{\partial\psi}{\partial\theta}\Big],$$

$$\mathcal{B}(x,t) = \Big[\Big(\frac{\partial K}{\partial\theta}\frac{\partial\theta}{\partial x} + \frac{\partial K}{\partial\phi_b}\frac{\partial\phi_b}{\partial x} + \frac{\partial K}{\partial b}\frac{\partial b}{\partial x}\Big)\frac{\partial\psi}{\partial\theta} + \Big(\frac{\partial K}{\partial\theta}\frac{\partial\psi}{\partial\phi_b}\frac{\partial\phi_b}{\partial x}\Big)$$
$$+ K(\theta,b,\phi_b)\frac{\partial}{\partial x}\Big(\frac{\partial\psi}{\partial\theta}\Big) + \frac{\partial K}{\partial\theta} + K(\theta,b,\phi_b)\frac{\partial^2\psi}{\partial\phi_b\partial\theta}\frac{\partial\phi_b}{\partial x}\Big],$$

$$\mathcal{C}(x,t) = \Big[K(\theta,b,\phi_b)\Big(\frac{\partial^2\psi}{\partial\phi_b^2}\Big(\frac{\partial\phi_b}{\partial x}\Big)^2 + \frac{\partial\psi}{\partial\phi_b}\frac{\partial^2\phi_b}{\partial x^2}\Big)$$
$$+ \Big(\frac{\partial K}{\partial b}\frac{\partial b}{\partial x} + \frac{\partial K}{\partial\phi_b}\frac{\partial\phi_b}{\partial x}\Big)\Big(1 + \frac{\partial\psi}{\partial\phi_b}\frac{\partial\phi_b}{\partial x}\Big) - h_2(\varepsilon f(c) - \phi_b)\phi_b\Big].$$

The following result concerns the solvability of the linear problem (3.48)–(3.51).

Proposition 3.5. *Consider $\theta \in V_3$ and $(\phi_b, b) \in V_1 \times V_2$. If the assumptions* (H.1)–(H.4) *are fulfilled then there exists $T^* > 0$ and a unique function $z \in C^{2+\alpha}(D_{T^*})$ solving the problem* (3.48)–(3.51).

Moreover,

$$0 < \Gamma_3 \leqslant z(x,t) \leqslant \varepsilon_0 - \delta - \Phi t, \quad \forall\,(x,t) \in D_{T^*}, \tag{3.52}$$

and

$$\|z\|_{2+\alpha} \leqslant p_7(R_1 + \overline{R}_2 + \overline{R}_3). \tag{3.53}$$

P r o o f. We note that, because of $\theta \in V_3$, we have

$$0 < \Gamma_3 \leqslant \theta \leqslant \varepsilon_0 - \delta - \Phi t,$$

so that the coefficients of the equation (3.48) are smooth and bounded. Moreover, $\mathcal{A}(x,t)$ is bounded and bounded away from zero, i.e. the equation is uniformly parabolic. Therefore, to the problem (3.48)–(3.51) we can apply Theorem 5.2, p. 320 of [4] giving the existence of a unique solution $z \in C^{2+\alpha}(D_T)$. The already quoted result of [4] gives us also the estimate

$$\|z\|_{2+\alpha} \leqslant p_6(\|\phi_b\|_{2+\alpha} + \|b\|_{1+\alpha} + \|\theta\|_{1+\alpha}),$$

and so

$$\|z\|_{2+\alpha} \leqslant p_7(R_1 + \overline{R}_2 + \overline{R}_3). \tag{3.54}$$

In particular, the estimate (3.54) entails

$$|z_t(x,t)| \leqslant p_7(R_1 + \overline{R}_2 + \overline{R}_3),$$

or

$$\Theta_{\min} - (R_1 + \overline{R}_2 + \overline{R}_3)t \leqslant z(x,t) \leqslant (R_1 + \overline{R}_2 + \overline{R}_3)t + \Theta_{\max},$$

with $\Theta_{\min} = \min\limits_{x\in(0,l)} \Theta_0(x)$ and $\Theta_{\max} = \max\limits_{x\in(0,l)} \Theta_0(x)$. Thus, defining t_1 as the first time in $(0,T]$ such that

$$\Theta_{\min} - (R_1 + \overline{R}_2 + \overline{R}_3)t_1 = \Gamma_3 \;\Leftrightarrow\; t_1 = \frac{\Theta_{\min} - \Gamma_3}{(R_1 + \overline{R}_2 + \overline{R}_3)}, \tag{3.55}$$

and t_2 as the first time in $(0,T]$ such that

$$\Theta_{\max} + (R_1 + \overline{R}_2 + \overline{R}_3)t_2 = \varepsilon_0 - \delta - \Phi t_2 \;\Leftrightarrow\; t_2 = \frac{\varepsilon_0 - \delta - \Theta_{\max}}{(R_1 + \overline{R}_2 + \overline{R}_3) + \Phi}, \tag{3.56}$$

we have that

$$\forall\,(x,t) \in (0,l) \times (0,T^*), \quad 0 < \Gamma_3 < z(x,t) < \varepsilon_0 - \delta - \Phi t,$$

with $T^* = \min(t_1, t_2)$, which is the estimate (3.52). □

The following proposition concerns an additional estimate for z.

Proposition 3.6. *The function $z \in C^{2+\alpha}(D_T)$ found in Proposition 3.5 satisfies the following estimate*

$$\|z\|_{1+\alpha} \leqslant p_{10}\|\Theta_0\|_{C^{2+\alpha}([0,l])} + p_{11}T^\gamma(R_1 + \|\Theta_l\|_{C^{1+\alpha}([0,T])}). \tag{3.57}$$

P r o o f. Let us consider the function

$$\omega(x,t) = \Theta_0(x) + \int_0^t \Big[\frac{\partial\varepsilon}{\partial t}(x,\tau)\Big(1 - \frac{x}{l}\Big) + x\frac{\partial\Theta_l}{\partial t}(\tau)\Big]\,\mathrm{d}\tau.$$

We have $\omega \in C^{2+\alpha}(D_T)$ and, thanks to the compatibility conditions on Θ_0 and Θ_l (see the assumption (H.4)),

$$\omega(x,0) = \Theta_0(x), \quad \omega(0,t) = \varepsilon(0,t), \quad \omega(l,t) = \Theta_l(t).$$

Moreover, we have

$$\|\omega\|_{1+\alpha} \leqslant \|\Theta_0\|_{C^{2+\alpha}([0,l])} + p_8T^\gamma(\|\phi_b\|_{2+\alpha} + \|\Theta_l\|_{C^{1+\alpha}([0,T])}). \tag{3.58}$$

Let us consider $\tilde{z}(x,t) = z(x,t) - \omega(x,t)$, which solves the problem

$$(P_{\tilde{z}}) \qquad \begin{cases} \dfrac{\partial \tilde{z}}{\partial t} = \mathcal{A}(x,t)\dfrac{\partial^2 \tilde{z}}{\partial x^2} + \mathcal{B}(x,t)\dfrac{\partial \tilde{z}}{\partial x} + \mathcal{D}(x,t), \\ \tilde{z}(x,0) = 0, \\ \tilde{z}(0,t) = 0 = \tilde{z}(l,t), \end{cases}$$

where

$$\mathcal{D}(x,t) = \mathcal{A}(x,t)\frac{\partial^2 \omega}{\partial x^2} + \mathcal{B}(x,t)\frac{\partial \omega}{\partial x} - \frac{\partial \omega}{\partial t} + \mathcal{C}(x,t) - \lambda b z.$$

To the problem $(P_{\tilde{z}})$ we apply the estimate (3.23) p. 200 of [3] giving

$$(3.59) \qquad \|\tilde{z}\|_{1+\alpha} \leqslant p_9 T^{\gamma}(\|\phi_b\|_{2+\alpha} + \|\Theta_0\|_{C^{2+\alpha}([0,l])} + \|\Theta_l\|_{C^{1+\alpha}([0,T])}).$$

Thus, exploiting (3.58) and (3.59), we have

$$\|z\|_{1+\alpha} \leqslant \|\tilde{z}\|_{1+\alpha} + \|\omega\|_{1+\alpha} \leqslant p_{10}\|\Theta_0\|_{C^{2+\alpha}([0,l])} + p_{11}T^{\gamma}(R_1 + \|\Theta_l\|_{C^{1+\alpha}([0,T])}),$$

namely the desired estimate (3.57). □

Proposition 3.7 (Continuous dependence for θ)**.** *In the framework of Proposition* 3.5, *if we consider* $(\theta_1, \theta_2) \in V_1$ *and the corresponding* z_1, z_2, *then we have*

$$(3.60) \qquad \|z_1 - z_2\|_{2+\nu} \leqslant r_5(\|\phi_{b,1} - \phi_{b,2}\|_{2+\nu} + \|b_1 - b_2\|_{2+\nu} + \|\theta_1 - \theta_2\|_{2+\nu})$$

where r_5 *is a positive constant depending on* $(D_b, h_2, B_{\max}, \phi_{\max}, c_0, \varepsilon_0, \lambda, \varrho, g, k_{\rm sat}^{(0)}, \mu_0 \cdot \psi_r, \delta, \alpha)$.

P r o o f. To prove (3.60) we add and subtract the appropriate terms in (3.48) and proceed as in the proof of Proposition 3.4. We omit the details. □

As a consequence of Propositions 3.5–3.7 we have the following theorem.

Theorem 3.2. *For a suitable choice of* $(R_1, R_2, R_3) \in \mathbb{R}^3$ *and* $\hat{T} > 0$, *there exists a solution* $(\phi_b, b, \theta, c) \in [C^{2+\alpha}(D_{\hat{T}})]^4$ *to the system* (2.7)–(2.18), *with* $(\phi_b, b, \theta) \in V_1 \times V_2 \times V_3$.

P r o o f. Let us consider a $\hat{T} > 0$ such that in $D_{\hat{T}}$ all the constraints given in Propositions 3.1–3.7 are satisfied. Then, consider $(\phi_b, b, \theta) \in V_1 \times V_2 \times V_3$ and the corresponding $z \in C^{2+\alpha}(D_{\hat{T}})$ given by Proposition 3.5. From the estimate (3.57) it is possible to choose T and $\overline{R}_3$ such that

$$\|z\|_{1+\alpha} \leqslant \overline{R}_3.$$

Once $\overline{R}_3$ is fixed, we consider the estimate (3.53) and look for R_3 such that

$$R_3 \geqslant p_7(\overline{R}_2 + \overline{R}_3) + p_7 R_1, \tag{3.61}$$

where $\overline{R}_2$ is given by (3.45). Finally, we have to check the possibility to choose a set (R_1, R_2, R_3) such that (3.61) is satisfied along with the constraint $(R_1, R_2) \in \mathcal{R}$, where $\mathcal{R}$ is the region defined by (3.46), (3.47).

It is elementary to show that (3.61) can always be made compatible with (3.46), (3.47) by reducing T if necessary (note that we can increase R_3, keeping the product TR_3 fixed).

Therefore, defining the mapping Λ on $V_3(R_3, \overline{R}_3)$ such that $\Lambda(\theta) = z$ and considering $(\phi_b, b) = \Lambda_\theta(\phi_b, b)$ the solution given by Theorem 3.1, we have

$$\Lambda(\theta) \in V_3(R_3, \overline{R}_3).$$

Moreover, Proposition 3.7 ensures the continuity of the mapping. On the other hand, we can exploit the same argument as in Theorem 3.1 to state the compactness of the space V_3. Therefore, the collection of these results implies that Λ is a completely continuous mapping and Schauder's theorem applies. This guarantees the existence of a fixed point $\theta \in V_3(R_3, \overline{R}_3)$ and the proof is complete. □

Remark 3.1. The existence result can be continued up to the possible occurrence of saturation somewhere in the domain. The mixed regime (saturated-unsaturated) would require different techniques and it is beyond the scope of this paper. On the contrary, the case of saturated flow is much simpler.

4. Considerations on the fluid media scaling

As stated in Section 1, the fluid media scaling is a technique to take into account the biomass effects on surface tension, contact angle and viscosity (see [7]). At the pore scale on the gas/liquid interface the capillary pressure $p_c = p_{\text{air}} - p_{\text{water}}$ is defined as

With no biomass	With biomass
$p_c = \dfrac{2\gamma_0 \cos\alpha_0}{R_0}$	$p_{c,\text{bio}} = \dfrac{2\gamma_{\text{bio}} \cos(\alpha_{\text{bio}})}{R_{\text{bio}}}$

where R_0, R_{bio} are the pore radii, γ_0, γ_{bio} are the surface tensions and α_0, α_{bio} are the contact angles, respectively. Making the fundamental assumption that the above relationship holds true also upon averaging the quantities on a R.E.V., i.e.

$$\frac{\langle p_{c,\text{bio}}\rangle}{\langle p_{c,0}\rangle} = \frac{\gamma_{\text{bio}}}{\gamma_0}\frac{\cos(\alpha_{\text{bio}})}{\cos\alpha_0}\frac{\langle R_0\rangle}{\langle R_{\text{bio}}\rangle},$$

we arrive at

$$\frac{p_{c,\mathrm{bio}}}{p_c} =: \Pi$$

where the quantity Π is a *scaling factor* for the capillary pressure, depending on the biomass concentration.

In the literature two methods are applied for exploiting the fluid media scaling approximation, namely:

(A) The simpler one consists in the following steps:

1. Solve the equation for the flow in case of no biomass and use the solution (i.e. the capillary pressure) in the differential system governing the pollutant and biomass evolution.
2. Finally, re-compute the capillary pressure as

$$p_{c,\mathrm{bio}} = \Pi p_c.$$

(B) An alternative method consists in the following procedure:

1. Rescaling first the capillary pressure $p_{c,\mathrm{bio}} = \Pi p_{c,0}$.
2. Using this rescaled pressure to solve the differential system for pollutant and biomass.

Using either method the numerical problem is strongly simplified. However, in any case there is an analytical drawback, since in general the re-scaled $p_{c,\mathrm{bio}}$ will not satisfy the equation for the flow (Richards' equation). We show this fact by the following counterexample.

4.1. A counterexample: steady saturated flow

Throughout this section we consider the very simple case of a steady saturated flow with a constant flux Q prescribed at the top surface. Moreover, for the sake of simplicity, we assume that the biomass affects only the liquid viscosity, namely we neglect the porosity variation. In this simplified framework, the scaling factor Π can be expressed as[3]

$$\Pi(b) = 1 - a_1 b + a_2 b^2, \tag{4.1}$$

where a_1 and a_2 are given constants.

Under the assumed conditions, Richards' equation reduces to

$$\frac{\partial}{\partial x} q(x) = 0.$$

[3] Here we use an approximation of the experimental law found in the literature (see [8], for instance), taking its expansion up to the second order.

In the case of no biomass, using the boundary conditions we get $q(x) \equiv Q$ so that

$$\psi^{(0)}(x) = \Big(Q\frac{\mu_0}{\varrho g k_{\text{sat}}} - 1\Big)x. \tag{4.2}$$

When the viscosity dependens on the biomass, we have

$$\psi(x) = \frac{Q}{\varrho g K_{\text{sat}}}\int_0^x \mu(b(\xi))\,\mathrm{d}\xi - x.$$

On the other hand, using the expression (2.2) we get

$$\psi(x) = \Big(\frac{Q\mu_0}{\varrho g K_{\text{sat}}} - 1\Big)x + \frac{Q\mu_0}{\varrho g K_{\text{sat}}}h_1\int_0^x b(\xi)\,\mathrm{d}\xi. \tag{4.3}$$

Now, the application of the fluid media scaling approach, type (A), consists in the following steps:

- Use $\theta = \theta(\psi^{(0)}(x))$ and $q(x) = Q$ to obtain a triple (c, b, ϕ_b).
- Re-scale the pressure head as $\psi_{\text{bio}}(x) = \Pi(b(x))\psi^{(0)}(x)$.

Recalling (4.2) and the expression (4.1) for $\Pi(b)$, we have

$$\psi_{\text{bio}}(x) = [1 - a_1 b(x) + a_2 b^2(x)]\Big(\frac{Q\mu_0}{\varrho g K_{\text{sat}}} - 1\Big)x, \tag{4.4}$$

so that, comparing (4.3) and (4.4) we easily see that the definition of $\psi_{\text{bio}}(x)$ matches the exact solution $\psi(x)$ only for specific choices of the constants.

In particular, we can prove this fact considering the approximation

$$b(x) \sim c_1 + c_2x^2 + c_3x^3 + \dots$$

where $c_1 = b(0)$.

After putting this expansion into (4.3) and (4.4), we equal the resulting expressions and get the following relationship,

$$\begin{aligned} Ah_1\Big[c_1x + c_2\frac{x^2}{2} + c_3\frac{x^3}{3} + \dots\Big] &= (A-1)x[(a_1c_1 + a_1c_2x + a_1c_3x^3 + \dots) \\ &\quad + a_2(c_1^2 + c_2^2x^2 + 2c_1c_2x + 2c_1c_3x^2 + \dots)^2] \\ &\quad + o(x^3). \end{aligned}$$

Now, matching the same powers of x we obtain the following linear system

$$\begin{cases} \Big(\dfrac{A}{A-1}\Big)h_1 = a_1 + (a_2c_1), \\ \Big(\dfrac{A}{A-1}\Big)\dfrac{h_1}{2} = a_1 + 2(a_2c_1), \end{cases}$$

from which, substituting the expression of A, we get a condition to be satisfied by a_2, i.e.

$$a_2 = -\Big(\frac{Q\mu_0}{Q\mu_0 - \varrho g K_{\rm sat}}\Big)\frac{h_1}{2b(0)}. \tag{4.5}$$

Therefore, the identity $\psi(x) = \psi_{\rm bio}(x)$ holds true *if and only if* the constant a_2 chosen in the definition of the scaling factor $\Pi = \Pi(b)$ satisfies the constraint (4.5).

This fact emphasises a weak point of the fluid media scaling procedure. As a matter of fact, (4.5) makes a physical constant, a_2, dependent on $b(0)$, thus on the data.

For the type (B) procedure a similar contradiction can be found.

References

[1] *M. Bause, P. Knabner*: Numerical simulation of contaminant biodegradation by higher order methods and adaptive time stepping. Comput. Vis. Sci. *7* (2004), 61–78. zbl
[2] *I. Borsi, A. Farina, A. Fasano, M. Primicerio*: Biomass growth in unsaturated porous media: hydraulic properties changes. Applied and industrial mathematics in Italy Ser. Adv. Math. Appl. Sci., Vol. 75. World Sci. Publ., Hackensack, 2007, pp. 196–207.
[3] *A. Friedman*: Partial Differential Equations of Parabolic Type. Prentice-Hall, Engelwood Cliffs, 1964. zbl
[4] *O. A. Ladyzhenskaya, V. A. Solonnikov, N. N. Ural'tseva*: Linear and Quasi-linear Equations of Parabolic Type. Translation of Mathematical Monographs, Vol. 23. American Mathematical Society (AMS), Providence, 1968. zbl
[5] *F. Maggi, A. Porporato*: Coupled moisture and microbial dynamics in unsaturated soils. Water Resour. Res. *43* (2007). zbl
[6] *W. Merz*: Global existence result of the Monod model. Adv. Math. Sci. Appl. *15* (2005), 709–726. zbl
[7] *E. E. Miller, R. D. Miller*: Physical theory for capillary flow phenomena. J. Appl. Phys. *27* (1956), 324–332.
[8] *M. L. Rockhold, R. R. Yarwood, M. R. Niemet, P. J. Bottomley, J. S. Selker*: Considerations for modeling bacterial-induced changes in hydraulic properties of variably saturated porous media. Adv. Wat. Res. *25* (2002), 477–495.
[9] *M. L. Rockhold, R. R. Yarwood, M. R. Niemet, P. J. Bottomley, J. S. Selker*: Experimental observations and numerical modeling of coupled microbial and transport processes in variably saturated sand. Vadose Zone J. *4* (2005), 407–417.

Authors' addresses: *I. Borsi*, *A. Farina*, *A. Fasano* (corresponding author), *M. Primicerio*, Dipartimento di Matematica "U. Dini", Università degli Studi di Firenze, Viale Morgagni 67/A, 50134 Firenze, Italy, e-mail: `fasano@math.unifi.it`.