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COMSOL MODELLING FOR A WATER INFILTRATION PROBLEM IN AN UNSATURATED MEDIUM

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Abstract

The paper deals with the COMSOL modelling of fluid diffusion in unsaturated porous media. A representative phenomenon in this class of problems is water infiltration in soils.

1 Introduction

The model we are concerned of describes the water infiltration into an isotropic, nonhomogeneous, unsaturated porous medium with a variable porosity. It consists of a diffusion equation with a transport term in addition with a initial data and a Dirichlet boundary condition

$$m(x)\frac{\partial u}{\partial t} - \Delta\beta^*(u) + \frac{\partial K(u)}{\partial x_3} = F \quad \text{in} \quad Q := \Omega \times (0,T), \tag{1}$$

$$m(x)u(x,0) = \theta_0(x) \quad \text{in} \quad \Omega, \tag{2}$$

$$u(x,t) = g(x) < u_s \quad \text{on} \quad \Sigma := \Gamma \times (0,T). \tag{3}$$

Key Words: boundary value problems for nonlinear parabolic PDE; stability and convergence of numerical methods; Flows in porous media.

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The domain Ω is an open bounded subset of $\mathbf{R}^3$, with the boundary $\Gamma := \partial\Omega$ piecewise smooth. We denote the space variable by $x := (x_1, x_2, x_3) \in \Omega$ and the time by $t \in (0, T)$, with T finite. The model is written in dimensionless form. The porosity is denoted by m, the function u stands for the water saturation, while by u_s we shall denote its maximum value.

The volumetric water content is given by mu and θ_0 is the initial volumetric water content.

2 Hypothesis

In the unsaturated case the diffusivity $\beta : (-\infty, u_s) \to [\rho, +\infty)$ is a continuous and monotonically increasing function that satisfies the following hypotheses:

(i_D) $\quad \beta(r) \geq \rho, \quad \beta(0) = \rho, \quad \forall r \in (-\infty, u_s),$

(ii_D) $\quad \lim\limits_{r \nearrow u_s} \beta(r) = +\infty,$

(iii_D) $\quad \lim\limits_{r \nearrow u_s} \int_0^r \beta(\xi) d\xi = +\infty.$

The function $K : (-\infty, u_s] \to [0, K_s]$ is a non-negative Lipschitz function satisfying the following condition

(i_k) there exists $M > 0$ such that

$$|K(r_1) - K(r_2)| \leq M |r_1 - r_2|, \quad \forall r_1, r_2 \in (-\infty, u_s],$$

and stands for the hydraulic conductivity.

We denote by β^* the primitive of the diffusivity β that vanishes at 0,

$$\beta^*(r) = \int_0^r \beta(\xi) d\xi, \quad \text{for} \quad r < u_s. \tag{4}$$

According to $(i_D) - (iii_D)$, β^* is a differentiable and a monotonically increasing function on $(-\infty, u_s)$ that satisfies:

(i) $\quad (\beta^*(r_1) - \beta^*(r_2))(r_1 - r_2) \geq \rho(r_1 - r_2)^2, \quad \forall r_1, r_2 \in (-\infty, u_s),$

(ii) $\quad \lim\limits_{r \nearrow u_s} \beta^*(r) = +\infty,$

(iii) $\quad \lim\limits_{r \nearrow u_s} \int_0^r \beta^*(\xi) d\xi = +\infty.$

We consider $\delta > 0$ and $g \in L^\infty(\Gamma)$ with $\|g(x)\|_{L^\infty(\Omega)} \leq u_s < u_s - \delta$. We assume $m \in C^1(\overline{\Omega})$ such that

$$0 < m_0 \leq m \leq \overline{m}, \tag{5}$$

for m_0 and $\overline{m}$ constants. In general, $\overline{m} = 1$.

Next we introduce a new function θ by $\theta(x,t) := m(x)u(x,t)$, thus we have $u = \frac{\theta}{m}$.

System (1)-(3) becomes

$$\frac{\partial\theta}{\partial t} - \Delta\beta^*\left(\frac{\theta}{m}\right) + \frac{\partial K\left(\frac{\theta}{m}\right)}{\partial x_3} = F \quad \text{in} \quad Q, \tag{6}$$

$$\theta(x,0) = \theta_0(x) \quad \text{in} \quad \Omega, \tag{7}$$

$$\theta(x,t) = m(x)g(x) := G(x) \quad \text{on} \quad \Sigma. \tag{8}$$

We assume that there exists w such that
(H_w) $\{w \in H^1(\Omega) \cap L^\infty(\Omega),\ \left\|\frac{w}{m}\right\|_{L^\infty(\Omega)} \leq u_s - \delta < u_s$ and $\frac{w}{m} = g|_\Gamma\}$.
By (i_D) and using the (H_w) property for w, we have

$$\rho < D\left(\frac{w}{m}\right) \leq \|D(y_s - \delta)\|_{L^\infty(\Omega)} := D_w < \infty. \tag{9}$$

By ϕ we denote the function

$$\phi := \theta - w \tag{10}$$

and observe that $\phi|_\Sigma = 0$.

Instead of problem (6)-(8) we have obtained a homogeneous Dirichlet boundary condition problem in ϕ

$$\frac{\partial\phi}{\partial t} - \Delta D_w(\phi) + \frac{\partial K\left(\frac{\phi+w}{m}\right)}{\partial x_3} = f \quad \text{in} \quad Q, \tag{11}$$

$$\phi(x,0) = \phi_0(x) = m(x)\theta_0(x) - w(x) \quad \text{in} \quad \Omega, \tag{12}$$

$$\phi(x,t) = 0 \quad \text{on} \quad \Sigma, \tag{13}$$

where

$$D_w(\phi) := \beta^*\left(\frac{\phi+w}{m}\right) - \beta^*\left(\frac{w}{m}\right)$$

and

$$f := F - \left(-\Delta\beta^*\left(\frac{w}{m}\right)\right).$$

It can be easily observed that $D_w(\phi)|_\Gamma = 0$.

3 Functional framework

Let V be $H_0^1(\Omega)$ endowed with the usual Hilbertian norm

$$\|\psi\|_V^2 = \int_\Omega |\nabla\psi|^2 \, dx, \quad \forall\psi \in V \tag{14}$$

and $V' = H^{-1}(\Omega)$ be its dual space. On V' we introduce the scalar product

$$\langle u, \overline{u}\rangle_{V'} = u(\psi) \qquad \forall u, \overline{u} \in V^{'}, \tag{15}$$

where $\psi \in V$ satisfies the boundary value problem:

$$-\Delta\psi = \overline{u}, \psi|_\Gamma = 0. \tag{16}$$

We introduce the operator $A : D(A) \subset V' \to V'$ by

$$\langle A\phi, \psi\rangle_{V',V} := \int_\Omega \left(\nabla D_w(\phi)\cdot\nabla\psi - K\left(\frac{\phi+w}{m}\right)\frac{\partial\psi}{\partial x_3}\right) dx, \, \forall\psi \in V, \tag{17}$$

where

$$D(A) := \{\phi \in L^2(\Omega) | \; D_w(\phi) \in V\}. \tag{18}$$

We have the Cauchy problem

$$\begin{aligned} \frac{d\phi}{dt} + A\phi &= f, \quad \text{a.e.} \quad t \in (0,T), \\ \phi(0) &= \phi_0. \end{aligned} \tag{19}$$

We define

$$j(r) = \begin{cases} \int_0^r m(\zeta)\beta^*(\zeta)d\zeta, & \text{for } r < u_s \\ +\infty, & \text{for } r \geq u_s. \end{cases}$$

Definition 1. Let $m \in C^1(\overline{\Omega})$, $F \in L^2(0,T;V')$, $j\left(\frac{\phi_0+w}{m}\right) \in L^1(\Omega)$ and (H_w) hold. By solution to (11)-(13) we mean a function

$$\phi \in C([0,T];L^2(\Omega)) \cap L^2(0,T;V)$$

such that $\frac{d\phi}{dt} \in L^2(0,T;V')$, $D_w(\phi) \in L^2(0,T;V)$ and

$$\left\langle \frac{d\phi}{dt}(t), \psi \right\rangle_{V',V} + \int_\Omega \left(\nabla D_w(\phi) \cdot \nabla \psi - K \left(\frac{\phi + w}{m} \right) \frac{\partial \psi}{\partial x_3} \right) dx \quad (20)$$

$$= \langle F(t), \psi \rangle_{V',V} \quad \text{a.e. } t \in (0,T),\ \forall \psi \in V,$$

$$\frac{\phi + w}{m} < u_s \text{ a.e. in } \Omega, \quad (21)$$

and $\phi(0) = \phi_0$ in Ω.

We notice that, if $F \in L^2(0,T;V')$, then $f \in L^2(0,T;V')$. Indeed, under hypothesis (H_w) we have

$$\left\| -\Delta \beta^* \left(\frac{w}{m} \right) \right\|_{V'} < \infty.$$

Now, if ϕ is a solution to (11)-(13), then $u = \frac{\phi + w}{m}$ is a solution to (1)-(3) belonging to the following spaces

$$u \in C([0,T]; L^2(\Omega)) \cap L^2(0,T; H^1(\Omega)) \quad (22)$$

$$\frac{du}{dt} \in L^2(0,T; (H^1(\Omega))'),\ \beta^*(u) \in L^2(0,T; H^1(\Omega)) \quad (23)$$

and

$$u < u_s \text{ a.e. on } \Omega. \quad (24)$$

4 Stability of the discretization scheme

Definition 2. Let $m \in C^1(\overline{\Omega})$, $f \in L^2(0,T;V')$ and $h > 0$ small enough be given. We take $D_A^h(0 = t_0 \leq t_1 \leq t_2 \leq ... \leq t_n; f_1^h, ..., f_n^h)$ an *h-discretization* on $[0,T]$ of the equation (19), for $h = \frac{T}{n}$ the time step and n the number of division points.

The functions f_i^h are computed as the time average of f within the interval $((i-1)h, ih)$, i.e.,

$$f_i^h := \frac{1}{h} \int_{(i-1)h}^{ih} f(s) ds, \quad i = 1, ..., n. \quad (25)$$

We remark that $f_i^h \in V'$ and are well defined, for any $\psi \in V$, by the relations

$$\left\langle f_i^h, \psi \right\rangle_{V',V} := \frac{1}{h} \int_{(i-1)h}^{ih} \langle f(s), \psi \rangle_{V',V}\, ds. \quad (26)$$

Definition 3. Let $m \in C^1(\overline{\Omega})$, $f \in L^2(0,T;V')$, $j\left(\frac{\phi_0+w}{m}\right) \in L^1(\Omega)$ and (H_w) hold. A solution to the h-discretization $D_A^h(0 = t_0 \leq t_1 \leq t_2 \leq ... \leq t_n; f_1^h, ..., f_n^h)$ is a piecewise constant function denoted $\phi^h : [0,T] \to V'$ whose values ϕ_i^h on $(t_{i-1}, t_i]$ satisfy the equations

$$\frac{\phi_i^h - \phi_{i-1}^h}{t_i - t_{i-1}} + A\phi_i^h = f_i^h, \quad i = 1, ..., n, \tag{27}$$

with

$$\phi^h(0) := \phi_0^h = \phi_0. \tag{28}$$

With these considerations we write the time discretized system (11)-(13) in the implicit form, as follows

$$\begin{aligned} \frac{\phi_i^h - \phi_{i-1}^h}{h} - \Delta D_w(\phi_i^h) + \frac{\partial K\left(\frac{\phi_i^h+w}{m}\right)}{\partial x_3} &= f_i^h \quad \text{in} \quad \Omega, \\ \phi_0^h &= \phi_0 \quad \text{in} \quad \Omega, \\ \phi_i^h &= 0 \quad \text{on} \quad \Gamma, \end{aligned} \tag{29}$$

for $i = 1, ..., n$.

Recalling the definition of the operator A we can write this in the abstract form

$$\left(\frac{1}{h}I + A\right)\phi_i^h = f_i^h + \frac{1}{h}\phi_{i-1}^h, \ i = 1, ..., n, \tag{30}$$

where I is the identity operator on V' and aim to prove that it has, for each i, a unique solution, ϕ_i^h, i.e.,

$$\left\langle \left(\frac{1}{h}I + A\right)\phi_i^h, \psi \right\rangle_{V',V} = \langle f_i^h, \psi \rangle_{V',V} + \left\langle \frac{1}{h}\phi_{i-1}^h, \psi \right\rangle_{V',V}, \tag{31}$$

for any $\psi \in V$, $i = 1, ..., n$.

The existence for problem (27)-(28) for h small enough follows by the quasi m-accretivity of the operator A, meaning the m-accretivity of the operator $\lambda I + A$, for λ large enough (see e.g., [4]), as we are going to prove below.

Proposition 4. Assume (i)-(iii), (i_K) and (H_w). Then the operator A is quasi - m-accretive.

The proof follows directly the definition of m-accretive operators. For more details we refer the reader to [2].

Proposition 5. Let (i)-(iii), (i_K) and (H_w) hold and assume

$$j\left(\frac{\phi_0 + w}{m}\right) \in L^1(\Omega), \tag{32}$$

$$f_i^h \in V',\ m \in C^1(\overline{\Omega}). \tag{33}$$

Then (30) has a unique solution $\phi_i^h \in D(A)$ and the discretization scheme is stable, i.e.,

$$\left\|\phi_p^h + w\right\|^2 \leq C,\ for\ any\ p = 1, ..., n, \tag{34}$$

$$h\sum_{i=1}^{p}\left\|D_w(\phi_i^h)\right\|_V^2 \leq C,\ for\ any\ p = 1, ..., n, \tag{35}$$

$$h\sum_{i=1}^{p}\left\|\frac{\phi_i^h - \phi_{i-1}^h}{h}\right\|_{V'}^2 \leq C,\ for\ any\ p = 1, ..., n, \tag{36}$$

where by C we have denoted some constants depending on the problem data and independent on p and h.

Proof. Since the operator A is quasi - m-accretive, then it follows that $\frac{1}{h}I + A$ is invertible and has a Lipschitz continuous inverse. Therefore, (30) has a unique solution $\phi_i^h \in D(A)$, meaning that $D_w(\phi_i^h) \in V$, which also implies that $\phi_i^h \in V$ for all $i = 1, ..., n$.

Next we shall establish the estimates to ensure the scheme stability.

For proving (35) we multiply (30) by $D_w(\phi_i^h) \in V$. We have

$$\begin{aligned} &\frac{1}{h}\int_\Omega \left(\phi_i^h - \phi_{i-1}^h\right) D_w(\phi_i^h)dx + \int_\Omega \left|\nabla D_w(\phi_i^h)\right|^2 dx \\ &= \left\langle f_i^h, D_w(\phi_i^h)\right\rangle_{V',V} + \int_\Omega K\left(\frac{\phi_i^h + w}{m}\right) \cdot \frac{\partial D_w(\phi_i^h)}{\partial x_3}dx. \end{aligned} \tag{37}$$

It follows that

$$\begin{aligned} &\frac{1}{h}\int_\Omega \left(j\left(\frac{\phi_i^h + w}{m}\right) - j\left(\frac{\phi_{i-1}^h + w}{m}\right)\right) dx + \left\|D_w(\phi_i^h)\right\|_V^2 \\ \leq\ &\frac{1}{k}\left\|D_w(\phi_i^h)\right\|_V^2 + k\left\|f_i^h\right\|_{V'}^2 + M^2 k\left\|\frac{\phi_i^h + w}{m}\right\|^2 \\ &+\frac{1}{h}\int_\Omega m\left|\beta^*\left(\frac{w}{m}\right)\right|\left|\frac{\phi_i^h + w}{m} - \frac{\phi_{i-1}^h + w}{m}\right| dx. \end{aligned} \tag{38}$$

After summing up from $i = 1$ to p and multiplying by h, we obtain

$$\begin{aligned}
& \int_\Omega j\left(\frac{\phi_p^h + w}{m}\right) dx + \left(1 - \frac{1}{k}\right) h \sum_{i=1}^{p} \left\| D_w(\phi_i^h) \right\|_V^2 \\
\leq \quad & M^2 kh \sum_{i=1}^{p} \left\| \frac{\phi_i^h + w}{m} \right\|^2 + kh \sum_{i=1}^{p} \left\| f_i^h \right\|_{V'}^2 + \int_\Omega j\left(\frac{\phi_0^h + w}{m}\right) dx \\
& + \beta_w \int_\Omega |w| \left| \frac{\phi_p^h + w}{m} \right| dx + \beta_w \int_\Omega |w| \left| \frac{\phi_0^h + w}{m} \right| dx.
\end{aligned} \tag{39}$$

The norm of f_i^h on V' satisfies

$$h \sum_{i=1}^{p} \left\| f_i^h \right\|_{V'}^2 \leq \sum_{i=1}^{n} \int_{(i-1)h}^{ih} \| f(s) \|_{V'}^2 \, ds = \int_0^T \| f(s) \|_{V'}^2 \, ds := C_f. \tag{40}$$

By the definition of the function j, it is easy to observe that

$$\int_\Omega j(r) dx \geq m_0 \frac{\rho}{2} r^2, \text{ for any } r \in \mathbf{R}.$$

We apply Lemma 2.5 (see [2]) for

$$\begin{aligned}
C_0 \quad : \quad & = \frac{2\overline{m}^2}{m_0 \rho} \left(kC_f + \int_\Omega j\left(\frac{\phi_0^h + w}{m}\right) dx + \frac{\rho}{4m_0} \left\| \phi_0^h + w \right\|^2 \right. \\
& \left. + \frac{2(\beta_w)^2}{m_0 \rho} \|w\|^2 \right), \\
C_M \quad : \quad & = \frac{2M^2 k}{m_0 \rho}
\end{aligned}$$

and obtain

$$\left\| \phi_p^h + w \right\|^2 \leq 2 \max\{1, C_M\} \left(\left\| \phi_0^h + w \right\|^2 + C_0 \right) e^{C_M T}, \tag{41}$$

for any $p = 1, ..., n$. Applying a result of the same lemma, we get

$$h \sum_{i=1}^{p} \left\| \phi_i^h + w \right\|^2 \leq h \max\left\{1, \frac{1}{C_M}\right\} e^{C_M T} \left((\phi_0^h + w) + C_0 \right). \tag{42}$$

Therefore, the right-hand sides in (41) and (42) are bounded by constants generically denoted C.

Plugging (42) in (39) we obtain for any $p = 1, ..., n$,

$$\begin{aligned} &\int_\Omega j\left(\frac{\phi_p^h+w}{m}\right)dx + \left(1-\frac{1}{k}\right)h\sum_{i=1}^{p}\left\|D_w(\phi_i^h)\right\|_V^2 \\ &\leq c(\rho, M, k, T, m_0, \overline{m})\left(\left\|\phi_0^h + w\right\|^2 + C_0\right), \end{aligned} \tag{43}$$

(where $c(\rho, M, k, T, m_0, \overline{m})$ is a constant depending on $\rho, M, k, T, m_0, \overline{m}$) and this leads to (35). By (41) we have actually obtained (34), as well.

We pass now to show (36). To this end we multiply (30) by

$$\delta\phi_i^h := \frac{\phi_i^h - \phi_{i-1}^h}{h}$$

scalarly in V' and multiply the result by h. We obtain

$$\begin{aligned} &\int_\Omega \left(j\left(\frac{\phi_i^h+w}{m}\right) - j\left(\frac{\phi_{i-1}^h+w}{m}\right)\right)dx + \left(1-\frac{1}{k}\right)h\left\|\delta\phi_i^h\right\|_{V'}^2 \\ \leq\ & kM^2h\left\|\frac{\phi_i^h+w}{m}\right\|^2 + kh\left\|f_i^h\right\|_{V'}^2 + \int_\Omega m\left|\beta^*\left(\frac{w}{m}\right)\right|\left|\frac{\phi_i^h+w}{m} - \frac{\phi_{i-1}^h+w}{m}\right|dx, \end{aligned}$$

and then we proceed exactly like before to deduce that

$$\int_\Omega j\left(\frac{\phi_p^h+w}{m}\right)dx + \left(1-\frac{1}{k}\right)h\sum_{i=1}^{p}\left\|\delta\phi_i^h\right\|_{V'}^2 \leq C, \tag{44}$$

whence (36) is proved. This ends the proof of Proposition 5. ∎

We stress that C denotes some constants depending on k, ρ, M, m_0, $\overline{m}$, the norms of f, ϕ_0 and w in the corresponding spaces and the domain Ω.

5 Numerical algorithm

For solving (31) (i.e., (29)) we consider an h-discretization of $[0, T]$ and denoting in (29)

$$\eta_i^h = \beta^*(\theta_i^h),\ G(\eta_i^h) := (\beta^*)^{-1}(\eta_i^h),\ K_G(\eta_i^h) := K(G(\eta_i^h)) \tag{45}$$

we are led to the transformed elliptic boundary value problem

$$\begin{aligned} mG(\eta_i^h) - h\Delta\eta_i^h + h\nabla\cdot K_G(\eta_i^h) &= \int_{t_{i-1}}^{t_i} f(s)ds + m\theta_{i-1}^h \quad \text{in } \Omega, \\ \eta_i^h &= h\phi_0 \quad \text{on } \Gamma, \end{aligned} \tag{46}$$

for each $i = 1, ..., n$, where

$$G(r) := (\beta^*)^{-1}(r). \tag{47}$$

For $i = 1$ we solve the system with $\theta_0^h = \theta_0$, we obtain θ_1^h from (46) and this becomes the new θ_{i-1}^h in the system for $i = 2$. The procedure is continued up to $i = n$. For each i, the semilinear elliptic system is solved by a COMSOL Multiphysics 3.4 package (see [6]). Then, having computed η_i^h, the solution θ_i^h is obtained as

$$\theta_i^h := (\beta^*)^{-1}(\eta_i^h). \tag{48}$$

The values θ_i^h represent the discrete values of the solution to (1)-(3) at the times $t_i = ih$.

Having the model (1)-(3) already written in dimensionless form, we shall perform numerical tests for a 2D case for

$$\beta(r) = \frac{1}{(1-r)^p}, \ \forall r, \ p \geq 1,$$

corresponding to a very fast diffusion. This case arises as a limit case of infiltration in porous media. Recently it has been found to reveal important diffusion features to dynamic population and biology flows.

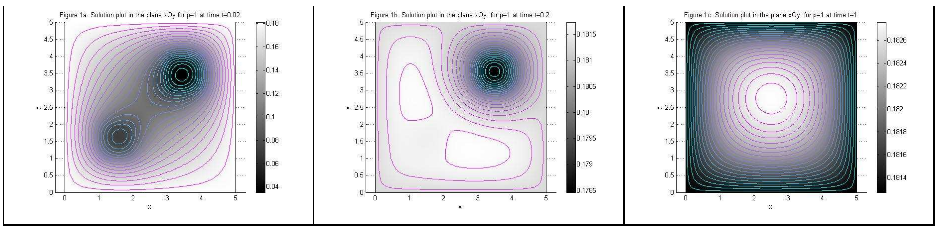
In what concerns K we consider it of the form

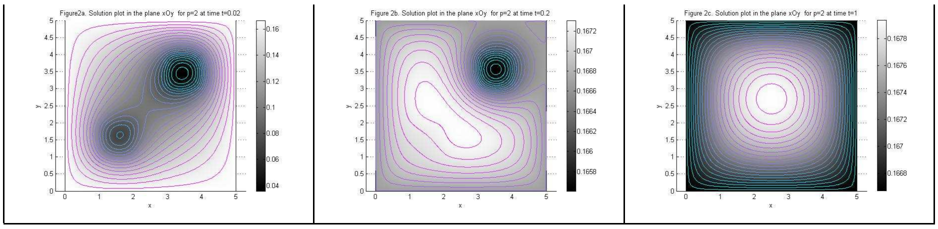
$$K(r) = r^2, \ \forall r. \tag{49}$$

The domain is a square defined by $\Omega = \{(x, y); x \in [0, 5], \ y \in [0, 5]\}$, Γ is the soil boundary and the the other data are

$$\begin{aligned} \theta_0(x, y) &= 0.1 \text{ for } x, y \in [2, 3], \ g(x) = 0.2, \ f(t, x, y) = 0.1, \\ m(x) &= \begin{cases} 0.1, & x, y \in [1, 2] \\ 0.2, & x, y \in [3, 4] \\ 0, & \text{otherwise.} \end{cases} \end{aligned}$$

System (46) was solved with Comsol Multiphysyics and Matlab (see [7]) for $i = 1, ...n$, with $h = 0.01$.





In these figures we represent the projection plots of the approximate solution θ^h in the plane xOy at three moments of time chosen in such a way to put into evidence the influence of $m(x, y)$. In (Fig.1a) and (Fig. 2a) we can observe the formation of two regions corresponding to the positive values of $m(x, y)$. The lighter areas correspond to higher values of the solution (higher moisture) and the dark areas indicate smaller ones. We observe that at small moments of time ($t = 0.2$ - figures b)), the region with the highest value of the porosity corresponds to small values for the moisture. At larger moments of time, the moisture moves towards the center of the domain. After $t = 1$, the solution becomes stationary.

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