

SOME FREE BOUNDARY PROBLEMS ARISING IN ROCK MECHANICS

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ABSTRACT. In the article we deal with some physical processes in rock mechanics, which are described by free-boundary problems. Some of them are well known (Muskat problems), some of them are completely new (in-situ leaching and dynamics of cracks in underground rocks).

CONTENTS

| | |
|--|-----|
| 1. Introduction | 492 |
| 2. Muskat Problem | 493 |
| 3. In-situ Leaching | 499 |
| 4. Dynamics of Cracks in Underground Rocks | 514 |
| References | 522 |

1. Introduction

The free-boundary problems are a subset of those partial differential equations devoted to initial boundary-value problems in unknown domains for different types of differential equations. The term unknown domain means that one must define the domain where the solution is to be found, together with a solution of the problem. To define this free boundary we need one more boundary condition for the same differential equations as compared with the regular boundary-value problem. This condition is usually called a *free boundary condition*. The systematic study of such problems for elliptic differential equations was initiated by Monakhov in [26], and for the heat equation (the Stefan problem) by Rubinstein [31]. Later, several books and papers mostly devoted to the Stefan problem [10, 20] have appeared.

The free-boundary problems for the Navier–Stokes equations have been intensively studied by Solonnikov [34, 35].

The most frequently studied free-boundary problems are the Stefan problem, the Hele–Shaw problem, and the Muskat problem. This is because these problems arise from physical processes, which are very important from a practical standpoint. For example, the Stefan problem describes phase transitions in pure materials (melting and solidification) and has many applications in metallurgy, and the Hele–Shaw and Muskat problems describe the motion of underground liquids and are very important for hydrology and oil industry. Among these three problems the Stefan problem is the most studied. This is confirmed by the fact that out of the free-boundary problems the Stefan problem has the largest number of publications.

On the other hand, from a practical point of view there are some very important physical processes in rock mechanics, which involve free boundaries, and which have been studied only by engineers. For example, in-situ leaching, and the dynamics of cracks in underground rocks. In-situ leaching initially involves drilling of holes into an ore deposit, then explosive or hydraulic fracturing may be used to create open pathways in the deposit for leaching solution to penetrate. The leaching solution is pumped into the deposit where it makes contact with the ore and dissolves part of it. The solution bearing the dissolved ore content is then pumped to the surface and processed. This method allows the extraction

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of metals and salts from an ore body without the need for conventional mining involving drill-and-blast, open-cut or underground mining. But existing mathematical descriptions of this process have been very primitive and involve some postulates about rock dissolution, which have no solid basis in classical continuum mechanics.

The latter problem, which we are going to study here, arises from the modeling of cracks in underground rocks. Up to now there has been no mathematical model of crack dynamics in underground rocks. For example, for metals this process is well studied [1]. Of course, this is an open question: is there any movement of cracks or not? But if there is, it may explain how many earthquakes occur [14]. In the rest state a single crack may be represented as a connected domain filled by pore fluids. During regular heat impulses, which come from the Earth's core, the stress on the boundary between fluid and solid skeleton grows up to some limit. After this limit the boundary of the crack starts to move (a moving free boundary) and creates strong seismic waves.

For the Muskat problem we first consider the motion of two different liquids in the pore space of a solid body and prove the existence and uniqueness of the classical solution. Next, under the restriction that the solid body has a periodic structure, we derive the homogenized model, which still remains a free-boundary problem.

We apply the same scheme for in-situ leaching and dynamics of cracks. We first derive mathematical models, describing the processes at the pore (microscopic) level, and after that we find corresponding homogenized models.

2. Muskat Problem

It is well known [32] that the Darcy system of filtration, describing the macroscopic flow of an incompressible viscous liquid, is a result of exact homogenization of the Stokes system for an incompressible viscous liquid occupying periodic pore space in an absolutely rigid solid body.

The more complicated macroscopic motion of two immiscible incompressible viscous liquids is governed by the Muskat problem. In this model one looks for the free boundary $\Gamma(t) \subset Q$, which separates two different domains $Q^+(t) \subset Q$ and $Q^-(t) \subset Q$, $Q^+(t) \cup \Gamma(t) \cup Q^-(t) = Q$, occupied by different fluids. In each of the domains $Q^\pm(t)$ the liquid motion is described by its own Darcy system of filtration, and at the free boundary the normal velocities of the liquids coincide with the normal velocity of the free boundary.

Thus, we may expect that, as in the case of the filtration of a single liquid, the Muskat problem should be a homogenization of the initial-boundary value problem for the Stokes system with a nonhomogeneous liquid

$$\mu \Delta \mathbf{u}^\varepsilon + g \rho_\varepsilon \mathbf{e} = 0, \quad \nabla \cdot \mathbf{u}^\varepsilon = 0, \quad \frac{d\rho_\varepsilon}{dt} = 0,$$

in a periodic pore space Q_ε of an absolutely rigid solid body Q with the following boundary and initial conditions

$$\mathbf{u}^\varepsilon(\mathbf{x}, t) = 0, \quad \mathbf{x} \in \partial Q_\varepsilon, \tag{2.1}$$

$$\rho_\varepsilon(\mathbf{x}, 0) = \rho_\varepsilon^0(\mathbf{x}), \quad \mathbf{x} \in Q_\varepsilon, \tag{2.2}$$

where $\rho_\varepsilon^0(\mathbf{x}) = \rho^+ = \text{const}$, $\mathbf{x} \in Q_\varepsilon^+(0)$, $\rho_\varepsilon^0(\mathbf{x}) = \rho^- = \text{const}$, $\mathbf{x} \in Q_\varepsilon^-(0)$, $\overline{Q_\varepsilon^+(0)} \cup \overline{Q_\varepsilon^-(0)} = \overline{Q_\varepsilon}$, μ is the viscosity and $g\mathbf{e}$ is the acceleration due to gravity.

Due to the boundary condition (2.1), the contact points of the free boundary and the solid skeleton will be permanently fixed at the initial position. Numerical implementations predict the appearance of a water tongue, which grows with time (see Fig. 2.1). The gradual growth of the number of capillaries (Fig. 2.2) leads to homogenization of the liquid motion. The domain occupied by the water tongues at a fixed time becomes under homogenization a mushy region, where the concentration s of water varies from 1 to 0 (Fig. 2.3 and Fig. 2.4).

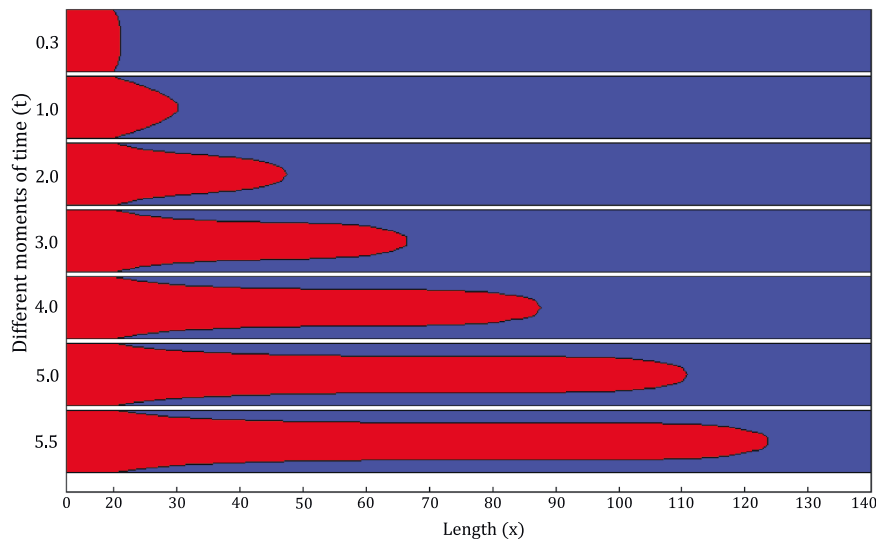


Fig. 2.1. Numerical simulation: successive positions of the free boundary in a single capillary

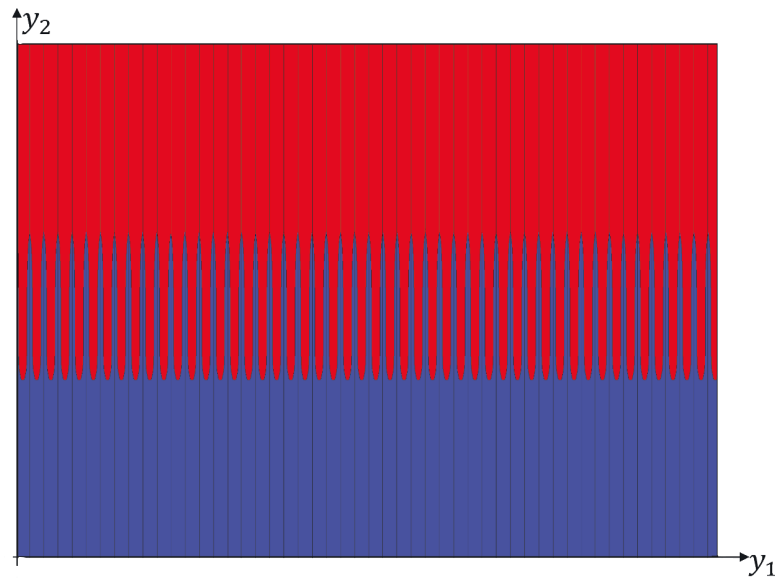


Fig. 2.2. Numerical homogenization for t=5.5

Now, if we return to the Muskat problem, we may see that the solution of the Muskat problem corresponding to the macroscopic joint motion of two different liquids has a very simple structure. The free boundary separates two liquids and moves with a constant velocity (Fig. 2.5).

Thus, we cannot obtain the Muskat problem of the liquid motion in the pore space of an absolutely rigid body as a homogenization of the corresponding initial-boundary value problem for a Stokes system with a nonhomogeneous liquid.

But, if we look at the motion of a nonhomogeneous liquid in an elastic solid body, then the situation changes. The contact points of the free boundary and solid body begin to move, and homogenization conserves the free boundary, which separates the two liquids [23].

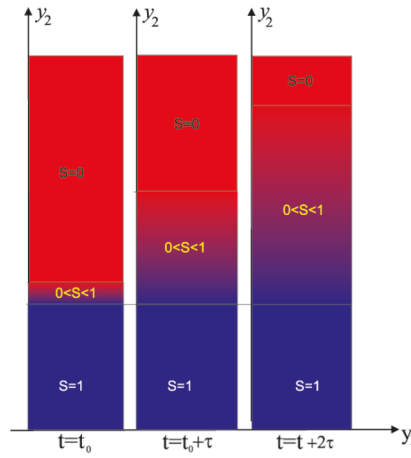


Fig. 2.3. Homogenization by increasing the number of capillaries. Concentration of water s for increasing times (left to right)

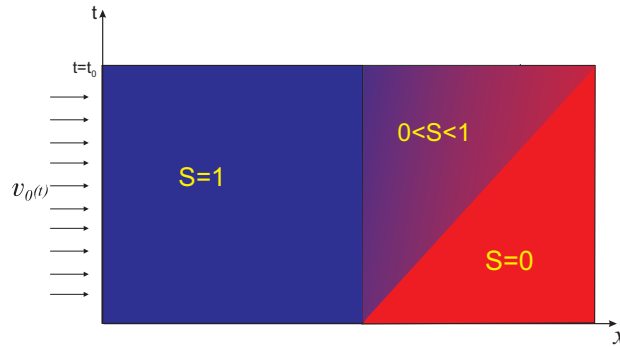


Fig. 2.4. The limit of rigorous numerical upscaling

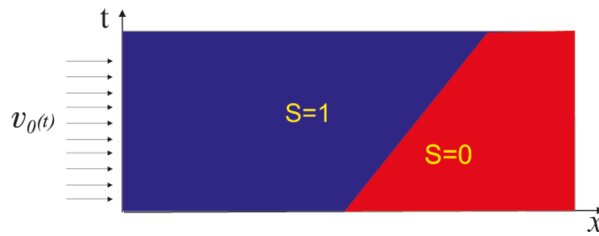


Fig. 2.5. The Muskat problem

Our approach does not depend on the dimension of the space \mathbb{R}^n and the geometry of domains there. Therefore, we restrict ourselves to \mathbb{R}^2 and to rectangles there. In its simplest setting the problem has the following statement.

Let $Q_f \subset Q \subset \mathbb{R}^2$, where Q is a unit square $Q = \{\mathbf{x} : -1 < x_i < 1, i = 1, 2\}$, $Q_f = \{\mathbf{x} : -1 < x_1 < 1, -\frac{1}{2} < x_2 < \frac{1}{2}\}$. In dimensionless variables the evolution of the flow is driven by the input pressure and the force of gravity. More precisely, in this problem one must find the velocity $\mathbf{u}^f(\mathbf{x}, t)$, pressure $p_f(\mathbf{x}, t)$, and density $\rho_f(\mathbf{x}, t)$ of the nonhomogeneous liquid in Q_f , and displacements $\mathbf{u}^s(\mathbf{x}, t)$ and pressure $p_s(\mathbf{x}, t)$ of an elastic skeleton in $Q_s = Q \setminus \overline{Q_f}$ from the following system of differential

equations

$$\begin{cases} \nabla \cdot \mathbb{P}_f + \rho_f \mathbf{e} = 0, \nabla \cdot \mathbf{u}^f = 0, \mathbf{x} \in Q_f, 0 < t < T, \\ \nabla \cdot \mathbb{P}_s + \rho_s \mathbf{e} = 0, \nabla \cdot \mathbf{u}^s = 0, \mathbf{x} \in Q_s, 0 < t < T, \end{cases} \quad (2.3)$$

$$\frac{d\rho_f}{dt} \equiv \frac{\partial \rho_f}{\partial t} + \nabla \cdot (\rho_f \mathbf{u}^f) = \frac{\partial \rho_f}{\partial t} + \mathbf{u}^f \cdot \nabla \rho_f = 0, \mathbf{x} \in Q_f, 0 < t < T, \quad (2.4)$$

where $\mathbb{P}_f = 2\mu \mathbb{D}(\mathbf{u}^f) - p_f \mathbb{I}$, $\mathbb{D}(\mathbf{u}^f) = \frac{1}{2}(\nabla \mathbf{u}^f + (\nabla \mathbf{u}^f)^*)$, $\mathbb{P}_s = 2\lambda \mathbb{D}(\mathbf{u}^s) - p_s \mathbb{I}$, $\mu = \text{const}$ is the viscosity of liquids, $\lambda = \text{const}$ is the Lamé's coefficient, \mathbf{e} is a given vector, ρ_s is the density of the solid body, and \mathbb{I} is the unit tensor.

The mass and momentum conservation laws dictate the coincidence of velocities and normal tensions of the liquid and solid components

$$\mathbf{u}^f = \frac{\partial \mathbf{u}^s}{\partial t}, \mathbb{P}_f \cdot \mathbf{n} = \mathbb{P}_s \cdot \mathbf{n} \quad (2.5)$$

on the common boundary $S = \partial Q_f \cap \partial Q_s$ with unit normal vector \mathbf{n} .

The boundary condition on the lateral part $S^0 = \{x_2 = \pm 1\}$ of the boundary ∂Q for $0 < t < T$ has the form

$$\mathbf{u}^s(\mathbf{x}, t) = 0. \quad (2.6)$$

At the "entrance" and "exit" boundaries $S^\pm = \{\mathbf{x} \in \partial Q : x_1 = \mp 1\}$

$$\begin{cases} \mathbb{P}_s \cdot \mathbf{e}_1 = -p^+(\mathbf{x})\mathbf{e}_1, \mathbf{x} \in S_s^+, \mathbb{P}_f \cdot \mathbf{e}_1 = -p^+(\mathbf{x})\mathbf{e}_1, \mathbf{x} \in S_f^+, 0 < t < T, \\ \mathbb{P}_s \cdot \mathbf{e}_1 = 0, \mathbf{x} \in S_s^-, \mathbb{P}_f \cdot \mathbf{e}_1 = 0, \mathbf{x} \in S_f^-, 0 < t < T, \end{cases} \quad (2.7)$$

where $p^+(\mathbf{x})$ is a given function, $S_f^\pm = S^\pm \cap \partial Q_f$, $S_s^\pm = S^\pm \cap \partial Q_s$, and \mathbf{e}_i is the unit vector of the x_i -axis for $i = 1, 2$.

To simplify our considerations, we pass to the homogeneous boundary conditions at S^\pm

$$\mathbb{P}_i \cdot \mathbf{e}_1 = 0, \mathbf{x} \in S_i^\pm, i = f, s, 0 < t < T, \quad (2.8)$$

by introducing a new pressure

$$p_f \rightarrow p_f - p^0(\mathbf{x}), \quad p^0(\mathbf{x}) = \frac{1}{2} p^+(\mathbf{x})(1 - x_1). \quad (2.9)$$

With this new pressure the dynamic equations take the form

$$\begin{cases} \nabla \cdot \mathbb{P}_f + \mathbf{f} + \rho_f \mathbf{e} = 0, \nabla \cdot \mathbf{u}^f = 0, \mathbf{x} \in Q_f, 0 < t < T; \\ \nabla \cdot \mathbb{P}_s + \mathbf{f} = 0, \nabla \cdot \mathbf{u}^s = 0, \mathbf{x} \in Q_s, 0 < t < T, \end{cases} \quad (2.10)$$

where

$$\mathbf{f}(\mathbf{x}) = (1 - \chi(\mathbf{x}))\rho_s \mathbf{e} + \nabla p^0(\mathbf{x}), \quad (2.11)$$

and

$$\chi(\mathbf{x}) = 1, \text{ for } \mathbf{x} \in Q_f, \text{ and } \chi(\mathbf{x}) = 0, \text{ for } \mathbf{x} \in Q_s.$$

Finally

$$\mathbf{u}^s(\mathbf{x}, 0) = 0, \mathbf{x} \in S^0. \quad (2.12)$$

The initial and boundary conditions for density are equivalent to specifying the surface Γ_0 that separates two subdomains $Q_f^\pm(0)$ initially occupied by different fluids. For the sake of simplicity we suppose that

$$\Gamma^{(0)} = \{\mathbf{x} \in Q_f : x_1 = h(x_2), -\frac{1}{2} < x_2 < \frac{1}{2}\}, \quad (2.13)$$

and

$$-\frac{1}{2} + \delta < h(x_2) < \frac{1}{2} - \delta, \text{ for } -\frac{1}{2} < x_2 < \frac{1}{2} \quad (2.14)$$

with some $0 < \delta < 1$.

Thus, we may expect that the free boundary $\Gamma(t)$ will not touch the given boundaries S^\pm , at least for some time interval $0 < t < T$.

At the boundaries S^\pm for $0 < t < T$ and at initial moment $t = 0$, the density ρ_f is piecewise constant and takes two positive values characterizing the distinct phases of the flow

$$\rho_f(\mathbf{x}, t) = \rho^\pm = \text{const} > 0, \quad \mathbf{x} \in S_f^\pm, \quad 0 < t < T, \quad (2.15)$$

$$\rho_f(\mathbf{x}, 0) = \rho_0(\mathbf{x}), \quad \mathbf{x} \in Q_f, \quad (2.16)$$

where $\rho_0(\mathbf{x}) = \rho^\pm$ for $\mathbf{x} \in Q_f^\pm(0)$.

Suppose for simplicity that $\rho^- \leq \rho_0(\mathbf{x}) \leq \rho^+$. If the velocity $\mathbf{u}^f(\mathbf{x}, t)$ is sufficiently smooth, then the Cauchy problem

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}^f(\mathbf{x}, t), \quad t > t_0, \quad \mathbf{x}|_{t=t_0} = \xi$$

determines a mapping $\mathbf{x} = \gamma(\xi, t; \mathbf{u}^f; t_0)$, $\gamma : Q_f \rightarrow Q_f$. In particular, the free boundary $\Gamma(t)$ is determined as a set $\Gamma(t) = \{\mathbf{x} \in Q_f : \mathbf{x} = \gamma(\xi, t; \mathbf{u}^f; 0), \xi \in \Gamma(0)\}$, and subdomains $Q_f^\pm(t) = \{\mathbf{x} \in Q_f : \rho_f(\mathbf{x}, t) = \rho^\pm\}$ as sets

$$Q_f^\pm(t) = \{\mathbf{x} \in Q_f : \mathbf{x} = \gamma(\xi, t; \mathbf{u}^f; 0), \xi \in Q_f^\pm(0)\} \cap \{\mathbf{x} \in Q_f : \mathbf{x} = \gamma(\xi, t; \mathbf{u}^f; t_0), \xi \in S_f^\pm, t_0 > 0\}.$$

It is shown that the evolution described by the above equations preserves the existence and uniqueness of two subdomains $Q_f^\pm(t)$, each occupied by one of the fluids, that are separated at time $t > 0$ by a regular free boundary $\Gamma(t)$. Thus, the problem studied is equivalent to finding $\{\mathbf{u}, p_f, \mathbf{w}, p_s\}$ and the moving boundary $\Gamma(t)$.

Throughout the section, we use the customary notation for function spaces and norms (see, e.g., [17]). Thus, for $1 < q < \infty$

$$u \in L_q(\Omega) \Rightarrow \|u\|_{q,\Omega} = \left(\int_{\Omega} |u|^q dx \right)^{\frac{1}{q}} < \infty, \quad u \in L_\infty(\Omega) \Rightarrow \|u\|_{\infty,\Omega} = \lim_{q \rightarrow \infty} \|u\|_{q,\Omega} < \infty,$$

$$u \in W_q^1(\Omega) \Rightarrow \|u\|_{q,\Omega}^{(1)} = \left(\int_{\Omega} |u|^q dx \right)^{\frac{1}{q}} + \sum_{i=1}^2 \left(\int_{\Omega} \left| \frac{\partial u}{\partial x_i} \right|^q dx \right)^{\frac{1}{q}} < \infty,$$

$$u \in \overset{\circ}{W}_q^1(\Omega) \Rightarrow u \in W_q^1(\Omega), \text{ and } u(\mathbf{x}) = 0, \quad \mathbf{x} \in \partial\Omega,$$

$$u \in W_q^l(\Omega) \Rightarrow \|u\|_{q,\Omega}^{(l)} = \left(\int_{\Omega} |u|^q dx \right)^{\frac{1}{q}} + \sum_{|m|=l} \left(\int_{\Omega} |D^m u|^q dx \right)^{\frac{1}{q}} < \infty,$$

$$D^m u = \frac{\partial^{|m|} u}{\partial^{m_1} x_1 \dots \partial^{m_n} x_n}, \quad m = (m_1, \dots, m_n), \quad m_i \geq 0, \quad |m| = m_1 + \dots + m_n.$$

Next we introduce the space of functions with noninteger derivatives. For simplicity, we consider half-spaces $\mathbb{R}_f^2 = \{\mathbf{x} = (x_1, x_2) \in \mathbb{R}^2 : |x_1| < \infty, x_2 > \frac{1}{2}\}$, $\mathbb{R}_s^2 = \{\mathbf{x} = (x_1, x_2) \in \mathbb{R}^2 : |x_1| < \infty, x_2 < \frac{1}{2}\}$, with the boundary $\mathbb{R} = \{\mathbf{x} \in \mathbb{R}^2 : |x_1| < \infty, x_2 = \frac{1}{2}\}$. The space $W_2^{l-\frac{1}{2}}(\mathbb{R})$ is the space of all functions $v(x_1)$ with the norm $\|v\|_{2,\mathbb{R}}^{(l-\frac{1}{2})} = \left(\int_{-\infty}^{\infty} |\xi|^{2l-1} |\widehat{v}(\xi)|^2 d\xi \right)^{\frac{1}{2}}$, where \widehat{v} is the Fourier transform of v :

$$\widehat{v}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} v(x_1) e^{-i\xi x_1} dx_1. \text{ By [17, Chap. 2, Theorem 2.3], } \|v\|_{2,\mathbb{R}}^{(l-\frac{1}{2})} \leq C_1 \|v\|_{2,\mathbb{R}^2}^{(l)} \leq C_2 \|v\|_{2,\mathbb{R}}^{(l-\frac{1}{2})},$$

$j = f, s.$

For smooth functions we define the following norms: $|u|_{\Omega}^{(0)} = \sup_{\mathbf{x} \in \Omega} |u(\mathbf{x})|$, $\langle u \rangle_{\Omega}^{(\alpha)} = \sup_{\mathbf{x}, \mathbf{y} \in \Omega} \frac{|u(\mathbf{x}) - u(\mathbf{y})|}{|\mathbf{x} - \mathbf{y}|^\alpha}$.

We say that a function $u(\mathbf{x})$ belongs to the space $C^\alpha(\overline{\Omega})$ if $|u|_{\Omega}^{(\alpha)} = |u|_{\Omega}^{(0)} + \langle u \rangle_{\Omega}^{(\alpha)} < \infty$; a function

$u(\mathbf{x})$ belongs to the space $C^k(\overline{\Omega})$ if $|u|_{\Omega}^{(k)} = \sum_{|m|=0}^k |D^m u|_{\Omega}^{(0)} < \infty$; and a function u belongs to the space $C^{k+\alpha}(\overline{\Omega})$ if $|u|_{\Omega}^{(k+\alpha)} = |u|_{\Omega}^{(k)} + \sum_{|m|=k} |D^m u|_{\Omega}^{(\alpha)} < \infty$. We say that the surface $\Gamma \in \Omega$ is $C^{k+\alpha}$ regular, if in local coordinates it is defined by $C^{k+\alpha}$ regular functions.

If $u = u(\mathbf{x}, t)$ and $u(\mathbf{x}, t) \in \mathbb{B}$ for all $0 < t < T$, then $u \in L_q((0, T); \mathbb{B}) \iff \int_0^T \|\mathbf{u}(\cdot, t)\|_B^q dt < \infty$, and for $q = \infty$ $u \in L_{\infty}((0, T); \mathbb{B}) \iff \sup_{0 < t < T} \|\mathbf{u}(\cdot, t)\|_B < \infty$.

Finally, $u \in C^{2,1}(\overline{\Omega_T})$, $\Omega_T = \Omega \times (0, T)$ if $\max_{0 < t < T} (|\mathbf{u}(\cdot, t)|_{\Omega}^{(2)} + |\frac{\partial u}{\partial t}(\cdot, t)|_{\Omega}^{(0)}) < \infty$.

For any $0 < \delta < 1$ we put $Q^{(\delta)} = \{\mathbf{x} \in Q : -1 + \delta < x_1 < 1 - \delta\}$, $Q_f^{(\delta)} = Q^{(\delta)} \cap Q_f$, $G^{(\delta)} = Q^{(\delta)} \times (0, T)$, $G_f = Q_f \times (0, T)$, $G_f^{(\delta)} = Q_f^{(\delta)} \times (0, T)$.

Our main result is the following theorem.

Theorem 2.1. *Under conditions*

$$\|\mathbf{f}\|_{\infty, Q} = C_0 < \infty, \quad \Gamma(0) \in C^{1+\alpha}, \quad 0 < \alpha < 1,$$

the problem (2.4)–(2.6), (2.8), (2.10), (2.12), (2.15), (2.16) has a unique solution in the interval $[0, T]$ for some $T > 0$.

The components of this solution possess the following properties.

- (i) For any $0 < \delta < 1$, and $0 < \alpha < 1$, the velocity \mathbf{u} and pressure p satisfy the regularity conditions $\mathbf{u} \in L_{\infty}(0, T; W_2^3(Q^{(\delta)})) \cap L_{\infty}(0, T; C^{1+\alpha}(Q^{(\delta)}))$, $p \in L_{\infty}(0, T; W_2^2(Q^{(\delta)}))$, equations (2.10) almost everywhere in $Q \times (0, T)$, boundary conditions (2.6), (2.15), and initial conditions (2.12) and (2.16) in the usual sense, and boundary conditions (2.5) and (2.8) in the sense of distributions as an integral identity $\int_{\Omega} (\mathbb{P}(\mathbf{u}(t), p(t)) : \mathbb{D}(\varphi) + \mathbf{f} \cdot \varphi) dx = 0$ for almost all $0 < t < T$ and for any smooth solenoidal functions φ vanishing at $\mathbf{x} \in S^0$.
- (ii) The free boundary $\Gamma(t)$ is a surface of class $C^{1,\alpha}$ at each time $t \in [0, T]$, and the normal velocity $V_n(\mathbf{x}, t)$ of the free boundary in the direction of its normal \mathbf{n} at position \mathbf{x} is uniformly bounded, $\sup_{\substack{t \in (0, T) \\ \mathbf{x} \in \Gamma(t)}} |V_n(\mathbf{x}, t)| < \infty$.
- (iii) The density ρ has bounded variation, $\rho \in L_{\infty}(0, T; BV(Q^{(\delta)})) \cap BV(Q^{(\delta)} \times (0, T))$, and satisfies the transport equation (2.4) in the sense of distributions as an integral identity $\int_{\Omega_T} \rho(\frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla \psi) dx dt = - \int_{\Omega} \rho_0(\mathbf{x}) \psi(\mathbf{x}, 0) dx$ for any smooth functions ψ , vanishing at $t = T$ and $\mathbf{x} \in S^{\pm}$.

The time T of the existence of the classical solution depends on the behavior of the free boundary $\Gamma(t)$. Namely, let $\delta^{\pm}(t)$ be the distance between $\Gamma(t)$ and the boundary S^{\pm} and $\delta(t) = \min(\delta^{-}(t), \delta^{+}(t))$. Then $\delta(t) > 0$ for all $0 < t < T$ and $\delta(t) \rightarrow 0$ as $t \rightarrow T$.

Theorems on the existence of generalized solutions to the Navier–Stokes system for nonhomogeneous incompressible fluids were obtained in e.g., [2, 4, 9, 11, 16, 17, 21, 29, 32, 33] (without detailed analysis of the set where the density is discontinuous). The existence and uniqueness of the classical solution to the Stokes equations for a nonhomogeneous liquid with Dirichlet boundary conditions have been proved in [3], and with the Neumann boundary conditions in [25]. The weak solutions to the problem (2.3)–(2.16) at the microscopic level for arbitrary smooth periodic pore space followed by homogenization was considered in [21]. Let us call the obtained homogenized free-boundary problem describing the motion of two immiscible incompressible viscous liquids at the macroscopic level as *the generalized Muskat problem*.

3. In-situ Leaching

3.1. Microscopic description.

3.1.1. *Mathematical model in the form of differential equations.* In dimensionless variables $\mathbf{x} \rightarrow \frac{\mathbf{x}}{L}$, $t \rightarrow \frac{t}{T}$, $\mathbf{v} \rightarrow \frac{T}{L} \mathbf{v}$, $p \rightarrow p^* p$, where L is the characteristic size of the domain $\Omega \subset \mathbb{R}^3$ under consideration, T is the characteristic time of the process, the behavior of liquid in the pore space $\Omega^f(t) \subset \Omega$ is described by the dynamic Stokes equation

$$\alpha_\mu \Delta \mathbf{v} - \nabla p = 0, \quad (3.1)$$

for the pressure p and the velocity \mathbf{v} of the liquid.

We will take a continuity equation in its generalized form [36], as the continuity equation of the generalized motion of the continuum media containing the solid skeleton $\Omega^s(t) \subset \Omega$, where $\mathbf{v} \equiv 0$, and the liquid in pores:

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho \chi \mathbf{v}) = 0. \quad (3.2)$$

Here χ is the characteristic function of the pore space: $\chi(\mathbf{x}, t) = 1$ in $\Omega^f(t)$ and $\chi(\mathbf{x}, t) = 0$ in $\Omega^s(t)$, $\Omega = \Omega^f(t) \cup \Gamma(t) \cup \Omega^s(t)$, $\Gamma(t) = \Omega^f(t) \cap \Omega^s(t)$.

The equation (3.2) is understood in the sense of distributions. For example, as an integral identity $\int_{\Omega_T} \varrho \left(\frac{\partial \varphi}{\partial t} + \chi \mathbf{v} \cdot \nabla \varphi \right) dx dt = 0$, $\Omega_T = \Omega \times (0, T)$ for the density $\varrho(\mathbf{x}, t) = \chi(\mathbf{x}, t) \varrho_f + (1 - \chi(\mathbf{x}, t)) \varrho_s$, which holds for any smooth $\varphi(\mathbf{x}, t)$, vanishing at S^+ , S^- , $t = 0$ and $t = T$.

In particular [36], $(v_n - d_n) \varrho_f = -d_n \varrho_s$, $\mathbf{x} \in \Gamma(t)$, $t > 0$, or

$$v_n = -d_n \delta, \quad \mathbf{x} \in \Gamma(t), \quad t > 0, \quad (3.3)$$

where d_n is the normal velocity of $\Gamma(t)$ in the direction of the outward to $\Omega^f(t)$ normal \mathbf{n} , and $v_n = \mathbf{v} \cdot \mathbf{n}$ is the normal liquid velocity.

Finally, the continuity equation in its differential form in the pore space $\Omega^f(t)$ for $t > 0$ takes the form

$$\nabla \cdot \mathbf{v} = 0. \quad (3.4)$$

The concentration c of the reagent is governed by the diffusion–convection equation

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = \alpha_c \Delta c, \quad (3.5)$$

and concentrations c_1, c_2, \dots, c_n of products of chemical reactions are governed by transport equations

$$\frac{\partial c_i}{\partial t} + \mathbf{v} \cdot \nabla c_i = 0, \quad i = 1, \dots, n \quad (3.6)$$

in $\Omega^f(t)$ for $t > 0$.

In (3.1)–(3.6) $\alpha_\mu = \frac{\mu}{T L g \rho^0}$, $\alpha_c = \frac{D T}{L^2}$, $p^* = L g \rho^0$, $\delta = \frac{(\varrho_s - \varrho_f)}{\varrho_f}$, μ is the fluid viscosity, $\chi(\mathbf{x}, t)$ is the characteristic function of the pore space ($\chi = 1$ in $\Omega^f(t)$ and $\chi = 0$ in $\Omega^s(t)$), ϱ_s and ϱ_f are dimensionless densities of the solid skeleton and the pore liquid correspondingly, correlated with the mean density of water ρ^0 , L is the characteristic size of the domain under consideration, T is the characteristic time of the process, g is the value of acceleration due to gravity, ρ_c is the density of the active component and D is a diffusivity coefficient.

Now we will try to formulate the basic boundary conditions for the concentrations c, c_1, c_2, \dots, c_n at the free boundary. First of all, we derive these conditions for one spatial variable.

Namely, let the pore space be given by $\Omega^f(t) = \{x : 0 < x < X(t)\}$ and $\Gamma(t) = \{x : x = X(t)\}$ be the free boundary (see Fig. 3.1).

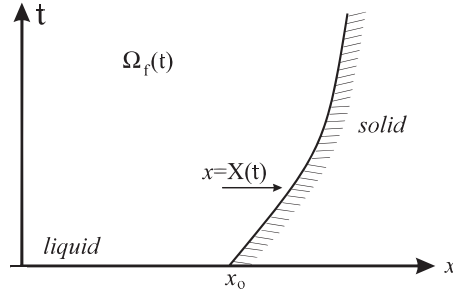


Fig. 3.1. One-dimensional structure

One has

$$\begin{cases} \frac{\partial v}{\partial x} = 0, & 0 < x < X(t), \\ \frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} = \alpha_c \frac{\partial^2 c}{\partial x^2}, & 0 < x < X(t), \\ \alpha_c \frac{\partial c}{\partial x} - v(t) c = 0 & \text{at } x = 0, \\ \frac{\partial c_i}{\partial t} + v \frac{\partial c_i}{\partial x} = 0, & 0 < x < X(t), \quad c_i = 0 \text{ at } x = 0, \quad i = 1, \dots, n. \end{cases} \quad (3.7)$$

Let $M(t) = \int_0^{X(t)} c(x, t) dx$, $M_i(t) = \int_0^{X(t)} c_i(x, t) dx$, $i = 1, \dots, n$ denote the total amounts of the concentration of the reagent c and the concentrations c_i , $i = 1, \dots, n$, of the products of chemical reactions in $\Omega^f(t)$.

First, we calculate the rate of change of these values in time:

$$\begin{aligned} \frac{dM}{dt} &= \frac{dX}{dt} c(X(t), t) + \int_0^{X(t)} \frac{\partial c}{\partial t}(x, t) dx = \frac{dX}{dt} c(X(t), t) + \int_0^{X(t)} \frac{\partial}{\partial x} (\alpha_c \frac{\partial c}{\partial x}(x, t) - v(t) c(x, t)) dx \\ &= \left(\frac{dX}{dt}(t) - v(t) \right) c(X(t), t) + \alpha_c \frac{\partial c}{\partial x}(X(t), t), \end{aligned}$$

$$\begin{aligned} \frac{dM_i}{dt} &= \frac{dX}{dt} c_i(X(t), t) + \int_0^{X(t)} \frac{\partial c_i}{\partial t}(x, t) dx = \frac{dX}{dt} c_i(X(t), t) - \int_0^{X(t)} v(t) \frac{\partial c_i}{\partial x}(x, t) dx \\ &= \left(\frac{dX}{dt}(t) - v(t) \right) c_i(X(t), t) = \frac{\rho_s}{\rho_f} \frac{dX}{dt} c_i(X(t), t), \quad i = 1, \dots, n. \end{aligned}$$

To calculate the integrals, we used integration by parts, the relation (3.3), and the boundary conditions in (3.7) at $x = 0$.

Thus,

$$\frac{dM}{dt} = \left(\frac{dX}{dt} - v \right) c + \alpha_c \frac{\partial c}{\partial x}, \quad \frac{dM_i}{dt} = \frac{\rho_s}{\rho_f} \frac{dX}{dt} c_i, \quad i = 1, \dots, n, \quad \text{at } x = X(t). \quad (3.8)$$

These relations mean that changes in the concentrations of the products of the chemical reactions occur only at $\Gamma(t)$. The values $\frac{dM}{dt}$, $\frac{dM_i}{dt}$, $i = 1, \dots, n$ are called the *rates of chemical reactions* and are defined additionally by the laws of chemical kinetics as:

$$\frac{dM}{dt} = -\beta c, \quad \frac{dM_i}{dt} = \beta \beta_i c, \quad i = 1, \dots, n, \quad (3.9)$$

where $\beta, \beta_i, i = 1, \dots, n$ are given constants.

On the other hand, the mass conservation law implies

$$\varrho_s \frac{dX}{dt} - \varrho_c \frac{dM}{dt} = \sum_{i=1}^n \varrho_i \frac{dM_i}{dt}, \quad (3.10)$$

where $\varrho_c, \varrho_1, \dots, \varrho_n$ are dimensionless densities of the reagent and the products of the chemical reactions.

The relations (3.8)–(3.10) result in

$$\frac{dX}{dt}(t) = \beta \gamma c(X(t), t), \quad c(X(t), t) \left(c_i(X(t), t) - c_i^0 \right) = 0, \quad i = 1, \dots, n, \quad (3.11)$$

and

$$\left(\frac{dX}{dt}(t) + \beta - v(t) \right) c(X(t), t) + \alpha_c \frac{\partial c}{\partial x}(X(t), t) = 0, \quad (3.12)$$

where $\varrho_s \gamma = \sum_{i=1}^n \varrho_i \beta_i - \varrho_c$, $c_i^0 = \frac{\varrho_f \beta_i}{\gamma \varrho_s}$, $i = 1, \dots, n$. Coming back to (3.4)–(3.6), we conclude that in the general case the mass conservation laws for the concentrations at the free boundary have the form

$$(d_n + \beta - v_n) c + \alpha_c \frac{\partial c}{\partial n} = 0, \quad \mathbf{x} \in \Gamma(t), \quad (3.13)$$

$$c(c_i - c_i^0) = 0, \quad i = 1, \dots, n, \quad \mathbf{x} \in \Gamma(t), \quad (3.14)$$

$$d_n = \beta \gamma c, \quad \mathbf{x} \in \Gamma(t), \quad (3.15)$$

where d_n is the normal velocity of $\Gamma(t)$ in the direction outward to $\Omega^f(t)$ normal \mathbf{n} , $v_n = \mathbf{v} \cdot \mathbf{n}$ is the normal liquid velocity, and $\frac{\partial c}{\partial n} = \nabla c \cdot \mathbf{n}$ is the normal derivative of c at $\Gamma(t)$.

It remains to supplement these differential equations by the missing *boundary conditions at the known boundaries* $S^\pm, S^0, \partial\Omega = S^+ \cup S^- \cup S^0$, and *at the free boundary* $\Gamma(t)$, and initial conditions.

At the free boundary $\Gamma(t)$, the tangent velocity of the pore liquid vanishes:

$$\mathbf{v} - v_n \mathbf{n} = 0. \quad (3.16)$$

At the boundaries S^\pm , which model the injecting (S^+) and the pumping (S^-) wells, we assume that the normal tension in the liquid is proportional to the given pressure

$$(2 \alpha_\mu \mathbb{D}(\mathbf{v}) - p \mathbb{I}) \cdot \mathbf{n} = -p^\pm(\mathbf{x}, t) \mathbf{n}, \quad (3.17)$$

where \mathbb{I} is the unit matrix, $p^\pm(\mathbf{x}, t) \mathbf{n}$ is the normal pressure and

$$\mathbb{D}(\mathbf{v}) = \frac{1}{2}(\nabla \mathbf{v} + \nabla \mathbf{v}^*).$$

At the injecting wells S^+ the concentrations of the reagent and the products of the chemical reactions are given by the quantities:

$$c = c^+(\mathbf{x}, t), \quad c_i = 0, \quad i = 1, \dots, n. \quad (3.18)$$

At the pumping wells S^- we have

$$\nabla c \cdot \mathbf{n} = 0, \quad (3.19)$$

and on the liquid impermeable boundary S^0 we obtain

$$\mathbf{v} = 0, \quad \nabla c \cdot \mathbf{n} = 0. \quad (3.20)$$

We add the following initial conditions to the problem:

$$\Gamma(0) = \Gamma_0, \quad c(\mathbf{x}, 0) = c_0(\mathbf{x}), \quad c_i(\mathbf{x}, 0) = 0, \quad i = 1, \dots, n, \quad \mathbf{x} \in \Omega_0. \quad (3.21)$$

The system of differential equations (3.1), (3.4), (3.5), and (3.6) completed with the boundary and initial conditions (3.3) and (3.13)–(3.21) forms the desired mathematical model, describing leaching at the pore scale.

Note that the problem (3.1), (3.3)–(3.5), (3.13), (3.15)–(3.18), (3.19)–(3.21) for the liquid velocity and the pressure, the concentration of the active admixture, and the free boundary is independent of the problem (3.6), (3.14), (3.18), (3.21) for the concentrations of the products of the chemical reactions.

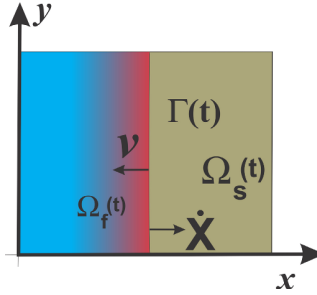


Fig. 3.2. One-dimensional motion

3.1.2. *Numerical implementations.* For the case of one spatial variable (see Fig. 3.2) the problem's differential equations (3.1)–(3.3), (3.21) for an incompressible liquid in the domain $0 < x < X(t)$ for $t > 0$ take the form

$$\begin{aligned}\frac{\partial p}{\partial x} &= 0, \\ \frac{\partial v}{\partial x} &= 0, \\ \frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} &= \alpha_c \frac{\partial^2 c}{\partial x^2}.\end{aligned}$$

Boundary and initial conditions (3.13)–(3.21) are transformed to

$$\begin{aligned}p(0, t) &= p^+(t), \quad c(0, t) = c^+(t), \quad t > 0, \\ \frac{dX}{dt} &= \beta \gamma c, \quad x = X(t), \quad t > 0, \\ \left(\frac{dX}{dt} + \beta - v\right) c + \alpha_c \frac{\partial c}{\partial x} &= 0, \quad x = X(t), \quad t > 0, \\ v(t) &= -\frac{dX}{dt}(t) \frac{(\rho_s - \rho_f)}{\rho_f}, \quad t > 0, \\ X(0) &= X_0, \quad c(x, 0) = c_0(x), \quad 0 < x < X_0.\end{aligned}$$

For $\gamma = 1$, $D = 2822 \frac{\mu m^2}{sec}$, $L = 50 \mu m$, $T = 1 sec$, and different values β and c^+ , we can calculate the concentration c of the reagent at the free boundary and the position of this boundary (see Fig. 3.3–3.6).

For the case of two spacial variables the system of differential equations in the domain $\Omega = \{0 < x_1 < L, 0 < x_2 < H\}$ (see Fig. 3.7) for the liquid velocity \mathbf{v} , liquid pressure p and concentration c of the reagent has the form

$$\begin{aligned}\alpha_\mu \Delta \mathbf{v} - \nabla p &= 0, \\ \nabla \cdot \mathbf{v} &= 0, \\ \frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c &= \alpha_c \Delta c.\end{aligned}$$

It is completed with boundary conditions at the free boundary $\Gamma(t)$ for $t > 0$:

$$(d_n + \beta - v_n) c + \alpha_c \frac{\partial c}{\partial n} = 0, \quad v_n = -d_n \delta, \quad \mathbf{v} - v_n \cdot \mathbf{n} = 0, \quad d_n = \beta \gamma c.$$

At the boundary S^+ , which models a well:

$$(2\alpha_\mu \mathbb{D}(\mathbf{v}) - p\mathbb{I}) \cdot \mathbf{n} = -p^+ \mathbf{n}, \quad c = c^+.$$

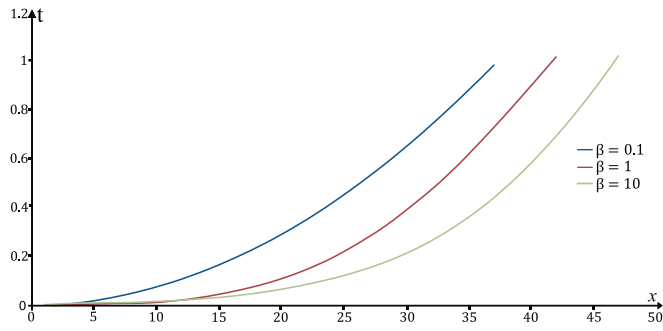


Fig. 3.3. Positions of the free boundary for different β

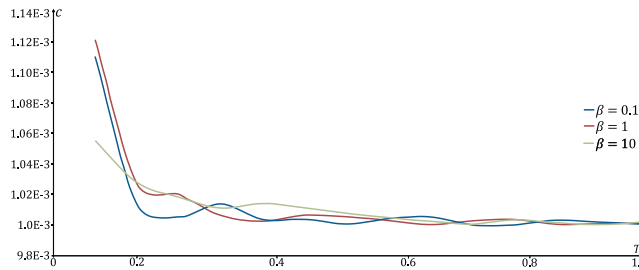


Fig. 3.4. Concentration of the reagent at the free boundary for different β

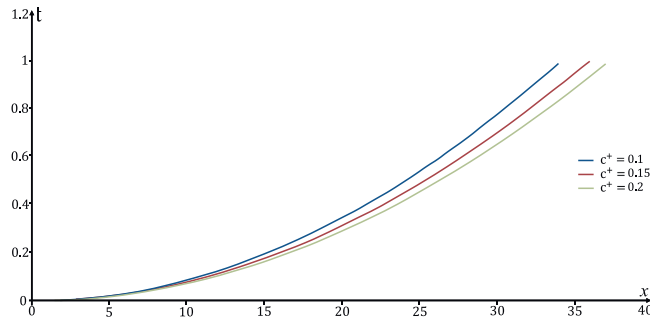


Fig. 3.5. Positions of the free boundary for different c^+

On the liquid impermeable boundary S^0 :

$$\mathbf{v} = 0, \quad \frac{\partial c}{\partial n} = 0.$$

The problem is ended with initial conditions

$$\Gamma(0) = \Gamma_0, \quad c(x, y, 0) = c_0(x, y), \quad (x, y) \in \Omega_0.$$

We have calculated the position of the free boundary and concentration of the reagent (see Fig. 3.10-3.11) for $D = 2822 \frac{\mu m^2}{sec}$, $L = 56 \mu m$, $H = 42 \mu m$, $T = 0.01 sec$, $\Gamma_0 = 14 \mu m$, $c_0 = 0$, $p^+ = 1000$, $\gamma = 1$, and different values β and c^+ (see Fig. 3.8-3.9).

In Fig. 3.8 the black line shows the initial position of the free boundary and colored lines show the positions of the free boundary at the moment $t = 0.01 sec$. for different $\beta = [0.1; 1; 5; 10]$.

In Fig. 3.9 the black line shows the initial position of the free boundary and colored lines show the positions of the free boundary at the moment $t = 0.01 sec$. for different $c^+ = [0.1; 0.3; 0.5; 0.7]$.

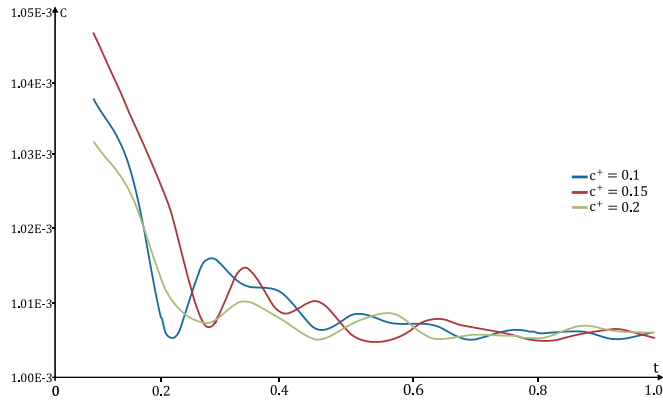


Fig. 3.6. Concentration of the reagent at the free boundary for different c^+

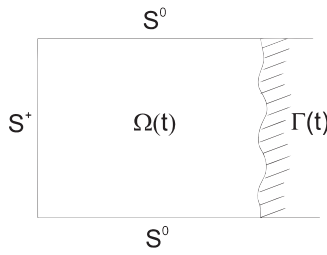


Fig. 3.7. Two-dimensional domain

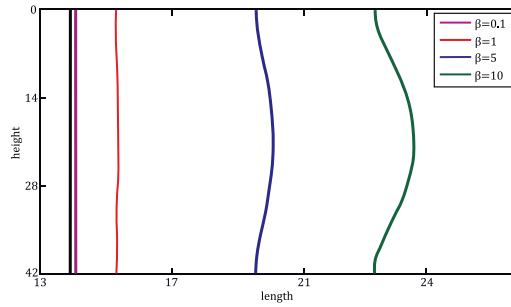


Fig. 3.8. Position of the free boundary for different β

3.2. Macroscopic description.

3.2.1. *Mathematical model as a system of integral identities.* Let $\chi(\mathbf{x}, t)$ be the characteristic function of the pore space: $\chi = 1$ in $\Omega^f(t)$ and $\chi = 0$ in $\Omega^s(t)$.

First of all, we introduce the new pressure $q = p - p^0(\mathbf{x}, t)$, where $p^0(\mathbf{x}, t) = p^\pm(\mathbf{x}, t)$ for $\mathbf{x} \in S^\pm$. With this new pressure the dynamic equation (3.1) and the boundary condition (3.9) take the form

$$\nabla \cdot (\alpha_\mu \mathbb{D}(\mathbf{v}, x)) - \nabla q = \mathbf{f} \equiv \nabla p^0, \quad \mathbf{x} \in \Omega^f(t), \quad 0 < t < t_0, \quad (3.22)$$

$$(\alpha_\mu \mathbb{D}(\mathbf{v}, x) - q \mathbb{I}) \cdot \mathbf{n} = 0, \quad \mathbf{x} \in S^\pm, \quad 0 < t < t_0. \quad (3.23)$$

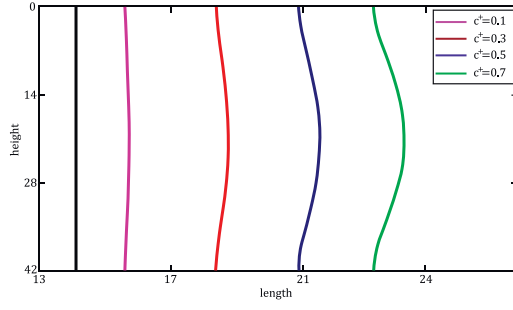


Fig. 3.9. Position of the free boundary for different c^+

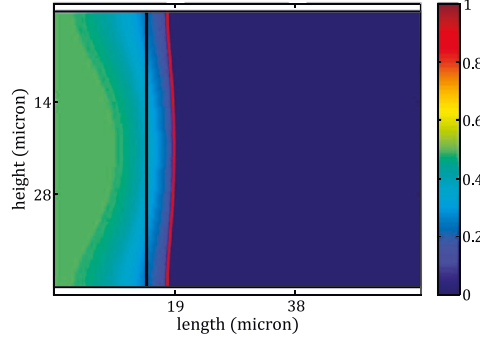


Fig. 3.10. The concentration of the reagent at $t=0.002$ sec.

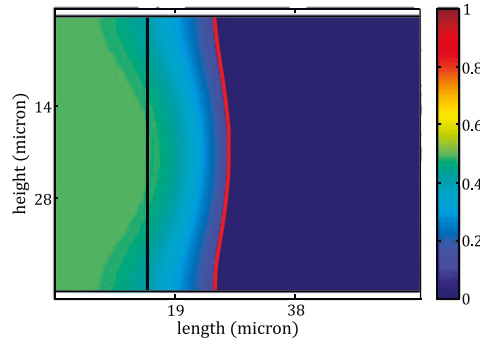


Fig. 3.11. The concentration of the reagent at $t=0.0052$ sec.

To get the integral identity for the velocity, we multiply Stokes equation (3.22) by arbitrary smooth function $\varphi(\mathbf{x}, t)$, vanishing at $\Gamma(t)$ and integrate over domain $\Omega^f(t)$

$$\int_{\Omega^f(t)} \left(\alpha_\mu \mathbb{D}(\mathbf{v}, x) : \mathbb{D}(\varphi, x) - q \nabla \cdot \varphi + \mathbf{f} \cdot \varphi \right) dx = 0, \quad (3.24)$$

$$\mathbb{D}(\mathbf{v}, x) = \frac{1}{2} (\nabla \mathbf{v} + (\nabla \mathbf{v})^*), \quad D_{ij}(\mathbf{v}, x) = \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right), \quad \text{and} \quad \mathbb{D}(\mathbf{v}, x) : \mathbb{D}(\varphi, x) = \sum_{i,j=1}^3 D_{ij}(\mathbf{v}, x) D_{ji}(\varphi, x).$$

The continuity equation (3.2) and boundary condition (3.3) are equivalent to the integral identity

$$\int_{\Omega_T} \left((\chi \rho_f + (1 - \chi) \rho_s) \frac{\partial \varphi}{\partial t} + \rho_f \mathbf{v} \cdot \nabla \varphi \right) dx dt = 0, \quad (3.25)$$

which is valid for arbitrary smooth function φ vanishing at the boundaries of S^+ and S^- at $t = 0$ and $t = t_0$. In (3.23) $\Omega_T = \Omega \times (0, T) \subset \mathbb{R}^4$.

The diffusion equation (3.5) together with the boundary conditions (3.13), (3.19), and the initial condition (3.21) is equivalent to the integral identity

$$\int_{\Omega_T} \chi \left(\left(c + \frac{1}{\gamma} \right) \frac{\partial \xi}{\partial t} - (\alpha_c \nabla c - \mathbf{v} c) \cdot \nabla \xi \right) dx dt = - \int_{\Omega} \chi_0(\mathbf{x}) \left(c_0(\mathbf{x}) + \frac{1}{\gamma} \right) \xi(\mathbf{x}, 0) dx, \quad (3.26)$$

which is valid for all smooth functions ξ vanishing at $t = t_0$ and on the boundaries of S^\pm .

Finally, transport equations (3.6) together with boundary and initial conditions (3.14), (3.21) are equivalent to the integral identities

$$\int_{\Omega_T} \chi \left(c_i \frac{\partial \psi}{\partial t} + \left(c_i - \frac{\rho_s c_i^0}{(\rho_s - \rho_f)} \right) \mathbf{v} \cdot \nabla \psi \right) dx dt = 0, \quad i = 1, \dots, n \quad (3.27)$$

for arbitrary smooth functions ψ , vanishing at the boundary S^- , and $t = t_0$.

To verify these identities we just reintegrate (3.26) and (3.27) using the Stokes theorem in the form

$$\begin{aligned} \int_{\Omega_T} \chi \left(A \frac{\partial \psi}{\partial t} + \mathbf{B} \cdot \nabla \psi \right) dx dt &= \int_0^T \int_{\Omega^f(t)} \left(A \frac{\partial \psi}{\partial t} + \mathbf{B} \cdot \nabla \psi \right) dx dt \\ &= - \int_0^T \int_{\Omega^f(t)} \psi \left(\frac{\partial A}{\partial t} + \nabla \cdot \mathbf{B} \right) dx dt + \int_0^T \int_{\Gamma(t)} \psi \left(\mathbf{B} \cdot \mathbf{n} - A d_n \right) \sin \omega \, d\sigma dt. \end{aligned}$$

Here $A(\mathbf{x}, 0) = 0$, \mathbf{n} is an outward to $\Omega^f(t)$ unit normal to $\Gamma(t)$ in \mathbb{R}^3 , ω is the angle between the outward unit normal ν to $\Gamma_T = \bigcup_{0 < t < T} \Gamma(t)$ in \mathbb{R}^4 and the time-axis t .

For example, to derive (3.27) we multiply the differential equation (3.6) by arbitrary smooth functions ψ , vanishing at the boundary S^- and $t = t_0$, integrate over Ω_{t_0} , use the Stokes theorem and boundary conditions (3.3), and (3.14) $\frac{\rho_s}{(\rho_s - \rho_f)} v_n = v_n - d_n$, and $c_i = c_i^0$, when we arrive at the integral over the boundary $\Gamma(t)$.

In fact,

$$\begin{aligned} 0 &= \int_{\Omega_T} \chi \psi \left(\frac{\partial c_i}{\partial t} + \mathbf{v} \cdot \nabla c_i \right) dx dt = \int_0^T \int_{\Omega^f(t)} \psi \left(\frac{\partial c_i}{\partial t} + \mathbf{v} \cdot \nabla c_i \right) dx dt \\ &= - \int_0^T \int_{\Omega^f(t)} c_i \left(\frac{\partial \psi}{\partial t} + \mathbf{v} \cdot \nabla \psi \right) dx dt + \int_0^T \int_{\Gamma(t)} \psi c_i (v_n - d_n) \sin \omega \, d\sigma dt \\ &= - \int_0^T \int_{\Omega^f(t)} c_i \left(\frac{\partial \psi}{\partial t} + \mathbf{v} \cdot \nabla \psi \right) dx dt + \int_0^T \int_{\Gamma(t)} \psi \frac{c_i^0 \rho_s}{(\rho_s - \rho_f)} v_n \sin \omega \, d\sigma dt \\ &= - \int_0^T \int_{\Omega^f(t)} c_i \left(\frac{\partial \psi}{\partial t} + \mathbf{v} \cdot \nabla \psi \right) dx dt + \int_0^T \int_{\Omega^f(t)} \frac{c_i^0 \rho_s}{(\rho_s - \rho_f)} \mathbf{v} \cdot \nabla \psi dx dt \end{aligned}$$

$$-\int_0^T \int_{\Omega^f(t)} \left(c_i \frac{\partial \psi}{\partial t} + \left(c_i - \frac{c_i^0 \rho_s}{(\rho_s - \rho_f)} \right) \mathbf{v} \cdot \nabla \psi \right) dx dt = \int_{\Omega_T} \chi \left(c_i \frac{\partial \psi}{\partial t} + \left(c_i - \frac{c_i^0 \rho_s}{(\rho_s - \rho_f)} \right) \mathbf{v} \cdot \nabla \psi \right) dx dt.$$

The system of integral identities (3.24)–(3.27), completed with boundary and initial conditions (3.15), (3.16), (3.18), (3.20), and (3.21) is equivalent to the initial setting (3.1), (3.3)–(3.6), (3.13)–(3.21) of the problem as a system of differential equations with corresponding boundary and initial conditions.

3.2.2. Homogenization. It is well known [32] that some of the limits in the integral identity (3.24) result from Darcy’s law

$$\mathbf{v} = -\frac{1}{\mu_1} \mathbb{B}(\nabla q + \mathbf{f}), \quad (3.28)$$

where $\mathbf{v}(\mathbf{x}, t) = \langle \mathbf{V} \rangle_Y \equiv \int_Y \mathbf{V}(\mathbf{x}, t, \mathbf{y}) dy$ and \mathbb{B} is a symmetric positive definite matrix.

In the case of liquid filtration Darcy’s law is usually supplemented with the standard continuity equation $\nabla \cdot \mathbf{v} = 0$. For our physical process of in-situ leaching Darcy’s law could be taken to be the same, while the continuity equation must take into account the dissolution of the rocks by leaching. This is why we choose a more accurate route from the exact description at the pore scale to the macroscopic description via homogenization. All homogenization methods assume the presence of a small parameter $\varepsilon > 0$. Roughly speaking, the homogenization itself consists of two parts: the study of the family of solutions to the mathematical problem depending on a small parameter ε , and the limiting procedure as the small parameter ε goes to zero.

Any physical problem contains dimensionless parameters (criteria), which somehow characterize the problem. Some of them might be small, some of them might be large, but all of them are fixed and we cannot let them be variable. On the other hand, when the physical problem has already been formulated as a mathematical problem, we may consider a family of mathematical problems with a variable small parameter and look for approximate mathematical models (homogenization), when this small parameter goes to zero.

For all physical problems in rock materials there is a natural small parameter, which is the ratio $\varepsilon_0 = \frac{l}{L}$, where l is the average pore size. Thus, in our physical problem describing in-situ leaching, we consider as the small parameter exactly this criterion.

Next, we formulate several assumptions, which enable us to obtain the mathematical setting of the in-situ leaching with a small parameter, and find some homogenized model, describing this procedure at the macroscopic level.

The main assumption is the behavior of dimensionless criteria

$$\alpha_\mu = \mu_1 \varepsilon^2 + o(\varepsilon^2), \quad \alpha_c = D_0 + o(\varepsilon), \quad (3.29)$$

where μ_1 and D_0 are some positive constants.

Next, we consider initial-boundary value problem (3.24)–(3.27), (3.10)–(3.12), with the given function $\chi = \chi^\varepsilon(\mathbf{x}, t) = \chi(\mathbf{x}, t, \frac{\mathbf{x}}{\varepsilon}) \equiv \chi(\mathbf{x}, t, \mathbf{y})$, which is 1-periodic in $\mathbf{y} \in Y = (0, 1)^3$, characterizing the solid pore space $\Omega^f(t)$, and let $\mathbf{v}^\varepsilon(\mathbf{x}, t)$, $q^\varepsilon(\mathbf{x}, t)$, $c^\varepsilon(\mathbf{x}, t)$, and $c_i^\varepsilon(\mathbf{x}, t)$, $i = 1, \dots, n$, be a solution of this problem.

For given function $\chi(\mathbf{x}, t, \mathbf{y})$ the problem (3.24)–(3.27), (3.10)–(3.12) has a unique solution $\mathbf{v}^\varepsilon(\mathbf{x}, t)$, $q^\varepsilon(\mathbf{x}, t)$, $c^\varepsilon(\mathbf{x}, t)$, and $c_i^\varepsilon(\mathbf{x}, t)$, $i = 1, \dots, n$.

Now, using the well-known formula (see [37]) for 1-periodic in \mathbf{y} function $\Phi(\mathbf{x}, t, \mathbf{y})$

$$\lim_{\varepsilon \rightarrow 0} \int_{\Omega_T} \Phi(\mathbf{x}, t, \frac{\mathbf{x}}{\varepsilon}) dx dt = \int_{\Omega_T} \left(\int_Y \Phi(\mathbf{x}, t, \mathbf{y}) dy \right) dx dt,$$

which expresses the notion of a two-scale convergence (see [22, 27, 28]), we pass to the limit as $\varepsilon \rightarrow 0$ in integral identities (3.24)–(3.27).

To do that, we choose some two-scale convergent subsequences $\{\mathbf{v}^{\varepsilon_k}(\mathbf{x}, t)\}$, $\{q^{\varepsilon_k}\}$, $\{c^{\varepsilon_k}(\mathbf{x}, t)\}$, and $\{c_i^{\varepsilon_k}(\mathbf{x}, t)\}$, $i = 1, \dots, n$, as $\varepsilon_k \rightarrow 0$ in the following sense

$$\begin{cases} \mathbf{v}^{\varepsilon_k}(\mathbf{x}, t) = \mathbf{V}(\mathbf{x}, t, \frac{\mathbf{x}}{\varepsilon_k}) + o(\varepsilon_k), & q^{\varepsilon_k}(\mathbf{x}, t) = q(\mathbf{x}, t) + o(\varepsilon_k), \\ c^{\varepsilon_k}(\mathbf{x}, t) = c(\mathbf{x}, t) + o(\varepsilon_k), & c_i^{\varepsilon_k}(\mathbf{x}, t) = c_i(\mathbf{x}, t) + o(\varepsilon_k), \\ \nabla c^{\varepsilon_k}(\mathbf{x}, t) = \nabla c(\mathbf{x}, t) + \nabla_y C(\mathbf{x}, t, \frac{\mathbf{x}}{\varepsilon_k}) + o(\varepsilon_k). \end{cases} \quad (3.30)$$

Here $\mathbf{V}(\mathbf{x}, t, \mathbf{y})$, $C(\mathbf{x}, t, \mathbf{y})$ are 1-periodic in \mathbf{y} functions.

3.2.3. Mathematical model in a form of differential equations. For the sake of simplicity in what follows we omit index k .

To get (3.28), we choose in (3.24) test functions of the form $\varphi = \zeta(\mathbf{x}, t)\varphi_0(\frac{\mathbf{x}}{\varepsilon})$, where $\varphi_0(\mathbf{y})$ is a solenoidal smooth function vanishing at $\gamma(t)$.

Here $\gamma(t)$ is a boundary between “liquid” and “solid” parts $Y_f = \{\mathbf{y} \in Y : \chi(\mathbf{x}, t, \mathbf{y}) = 1\}$ and $Y_s = \{\mathbf{y} \in Y : \chi(\mathbf{x}, t, \mathbf{y}) = 0\}$.

After that, using representations (3.29) and (3.30), one arrives at the integral identity

$$\begin{aligned} 0 &= \int_{\Omega_T} \zeta(\mathbf{x}, t) \chi^\varepsilon \left(\alpha_\mu \mathbb{D}(\mathbf{v}^\varepsilon, x) : \mathbb{D}(\varphi_0, x) \right) + (\nabla q^\varepsilon + \mathbf{f}) \cdot \varphi_0\left(\frac{\mathbf{x}}{\varepsilon}\right) dxdt + o(\varepsilon) \\ &= \int_{\Omega_T} \zeta(\mathbf{x}, t) \chi^\varepsilon \left(\varepsilon^2 \mu_1 \mathbb{D}(\mathbf{V}(\mathbf{x}, t, \frac{\mathbf{x}}{\varepsilon}), x) : \mathbb{D}(\zeta(\mathbf{x}, t)\varphi_0(\frac{\mathbf{x}}{\varepsilon})) + \mathbf{f} \cdot \varphi_0\left(\frac{\mathbf{x}}{\varepsilon}\right) \right) dxdt \\ &\quad + \int_{\Omega_T} \zeta(\mathbf{x}, t) \chi^\varepsilon \nabla q \cdot \varphi_0\left(\frac{\mathbf{x}}{\varepsilon}\right) dxdt + o(\varepsilon) = I_1 + I_2 + o(\varepsilon). \end{aligned}$$

It is easy to see that $I_1 \rightarrow \int_{\Omega_T} \zeta(\mathbf{x}, t) \left(\int_{Y_f} (\mu_1 \mathbb{D}(\varphi_0(\mathbf{y}), y) : \mathbb{D}(\mathbf{V}(\mathbf{x}, t, \mathbf{y}), y) + \mathbf{f} \cdot \varphi_0(\mathbf{y})) dy \right) dxdt$, and

$$\begin{aligned} I_2 &= \int_{Q_T} \zeta \chi^\varepsilon \nabla q \cdot \varphi_0\left(\frac{\mathbf{x}}{\varepsilon}\right) dxdt = \int_0^T \int_{\Omega^f(t)} \zeta \nabla q \cdot \varphi_0\left(\frac{\mathbf{x}}{\varepsilon}\right) dxdt \\ &= - \int_0^T \int_{\Omega^f(t)} q \nabla \zeta \cdot \varphi_0\left(\frac{\mathbf{x}}{\varepsilon}\right) dxdt = - \int_{Q_T} \chi^\varepsilon q \nabla \zeta \cdot \varphi_0\left(\frac{\mathbf{x}}{\varepsilon}\right) dxdt \rightarrow - \int_{\Omega_{t_0}} q \nabla \zeta \cdot \left(\int_Y \chi(\mathbf{x}, t, \mathbf{y}) \varphi_0(\mathbf{y}) dy \right) dxdt \\ &= \int_{\Omega_T} \zeta \nabla q \cdot \left(\int_Y \chi(\mathbf{x}, t, \mathbf{y}) \varphi_0(\mathbf{y}) dy \right) dxdt = \int_{\Omega_T} \zeta \left(\int_Y \chi(\mathbf{x}, t, \mathbf{y}) \nabla q \cdot \varphi_0(\mathbf{y}) dy \right) dxdt \end{aligned}$$

as $\varepsilon \rightarrow 0$.

Thus,

$$\begin{aligned} 0 &= \int_{\Omega_T} \zeta(\mathbf{x}, t) \left(\int_Y \chi(\mathbf{x}, t, \mathbf{y}) \left(\mu_1 \mathbb{D}(\varphi_0(\mathbf{y}), y) : \mathbb{D}(\mathbf{V}(\mathbf{x}, t, \mathbf{y}), y) + (\nabla q + \mathbf{f}) \cdot \varphi_0(\mathbf{y}) \right) dy \right) dxdt \\ &= \int_{\Omega_T} \zeta(\mathbf{x}, t) \left(\int_{Y_f} \varphi_0(\mathbf{y}) \left(-\mu_1 \nabla_y \cdot \mathbb{D}(\mathbf{V}(\mathbf{x}, t, \mathbf{y}), y) + \nabla q + \mathbf{f} \right) dy \right) dxdt \end{aligned}$$

$$\begin{aligned}
&= \int_{\Omega_T} \zeta(\mathbf{x}, t) \left(\int_{Y_f} \varphi_0(\mathbf{y}) \left(-\frac{\mu_1}{2} \Delta_y \mathbf{V}(\mathbf{x}, t, \mathbf{y}) + \nabla q + \mathbf{f} \right) dy \right) dxdt \\
&= \int_{\Omega_T} \zeta(\mathbf{x}, t) \left(\int_{Y_f} \varphi_0(\mathbf{y}) \left(-\frac{\mu_1}{2} \Delta_y \mathbf{V}(\mathbf{x}, t, \mathbf{y}) + \nabla q + \mathbf{f} \right) dy \right) dxdt = 0.
\end{aligned}$$

Due to the arbitrary choice of $\zeta(\mathbf{x}, t)$ and $\varphi_0(\mathbf{y})$ the latter identity results in the following differential equation

$$-\frac{\mu_1}{2} \Delta_y \mathbf{V} + \nabla_y Q + \nabla q + \mathbf{f} = 0 \quad (3.31)$$

in the domain Π_f .

The term $\nabla_y Q(\mathbf{x}, t, \mathbf{y})$ in (3.31) appears because of the orthogonality of solenoidal vectors to the gradients of scalar functions.

To solve this equation, we need boundary conditions for \mathbf{V} on the boundary γ , separating Y_f and its open supplement Y_s in Π : $\gamma = \partial\Pi_f \cap \partial\Pi_s$. We do not need a boundary condition for \mathbf{V} on the other part of $\partial\Pi_f$ because of the periodicity of \mathbf{V} in \mathbf{y} .

The desired boundary condition

$$\mathbf{V} = 0, \mathbf{y} \in \gamma \quad (3.32)$$

follows from the identity $\mathbf{V}(\mathbf{x}, t, \mathbf{y})(1 - \chi(\mathbf{x}, t, \mathbf{y})) = 0$, $\mathbf{y} \in Y$, which, in turn, is the result of the two-scale convergence in the evident identity $\mathbf{v}^\varepsilon(\mathbf{x}, t)(1 - \chi(\mathbf{x}, t, \frac{\mathbf{x}}{\varepsilon})) = 0$, $\mathbf{x} \in Y$.

To derive the microscopic continuity equation, we pass to the limit as $\varepsilon \rightarrow 0$ in the integral identity (3.25) with test functions $\varphi = \varepsilon \varphi_0(\mathbf{x}, t) \varphi_1(\frac{\mathbf{x}}{\varepsilon})$, where φ_0 are arbitrary smooth functions in variables \mathbf{x} and t vanishing at $t = 0$ and $t = T$, and $\varphi_1(\mathbf{y})$ is a 1-periodic in \mathbf{y} smooth function vanishing at γ :

$$\begin{aligned}
0 &= \int_{\Omega_T} ((\chi^\varepsilon \rho_f + (1 - \chi^\varepsilon) \rho_s) \frac{\partial \varphi}{\partial t} + \rho_f \mathbf{v}^\varepsilon \cdot \nabla_x \varphi) dxdt \\
&= \int_{\Omega_T} \varphi_0(\mathbf{x}, t) \rho_f \mathbf{V}(\mathbf{x}, t, \frac{\mathbf{x}}{\varepsilon}) \cdot \nabla_y \varphi_1 dxdt + o(\varepsilon) \rightarrow \int_{\Omega_T} \varphi_0(\mathbf{x}, t) \left(\int_Y \rho_f \mathbf{V}(\mathbf{x}, t, \mathbf{y}) \cdot \nabla_y \varphi_1 dy \right) dxdt = 0.
\end{aligned}$$

The arbitrary choice of functions φ_0 and φ_1 results in the microscopic continuity equation

$$\nabla \cdot \mathbf{V} = 0 \quad (3.33)$$

in Y_f .

3.3. Darcy's law. Let $\mathbf{v}(\mathbf{x}, t) = \langle \mathbf{V} \rangle = \int_Y \mathbf{V}(\mathbf{x}, t, \mathbf{y}, \tau) dy$ and $\frac{2}{\mu_1}(\nabla q + \mathbf{f}) = \sum_{i=1}^3 z_i(\mathbf{x}, t) \mathbf{e}_i$, where $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ is the standard orthogonal Cartesian basis in \mathbb{R}^3 .

To find representation (3.28) for the liquid velocity \mathbf{v} in terms of microstructure, we solve the problem (3.31), (3.32), (3.33) using decomposition $\mathbf{V}(\mathbf{x}, t, \mathbf{y}, \tau) = \sum_{i=1}^3 \mathbf{V}^i(\mathbf{y}) z_i(\mathbf{x}, t)$. The functions $\mathbf{V}^i(\mathbf{y})$ and $Q^i(\mathbf{y})$ for $i = 1, 2, 3$ satisfy in Y_f the following periodic boundary-value problems

$$-\Delta_y \mathbf{V}^i + \nabla_y Q^i + \mathbf{e}_i = 0, \mathbf{y} \in Y_f, \quad (3.34)$$

$$\nabla \cdot \mathbf{V}^i = 0, \mathbf{y} \in Y_f, \quad (3.35)$$

$$\mathbf{V}^i = 0, \mathbf{y} \in \gamma. \quad (3.36)$$

Therefore,

$$\mathbf{v} = \sum_{i=1}^3 \mathbf{V}^i(\mathbf{y}) z_i = -\frac{2}{\mu_1} \left(\sum_{i=1}^3 \mathbf{V}^i \otimes \mathbf{e}_i \right) (\nabla q + \mathbf{f}). \quad (3.37)$$

Here $\mathbf{a} \otimes \mathbf{b}$ is a matrix of order 2, which is defined as $(\mathbf{a} \otimes \mathbf{b}) \cdot \mathbf{c} = \mathbf{a}(\mathbf{b} \cdot \mathbf{c})$. Coming back to (3.28), we get

$$\mathbf{v} = \sum_{i=1}^3 \langle \mathbf{V}^i \rangle_Y z_i = -\frac{1}{\mu_1} \mathbb{B} \cdot (\nabla q + \mathbf{f}), \quad (3.38)$$

where

$$\mathbb{B} = 2 \sum_{i=1}^3 \langle \mathbf{V}^i \rangle_Y \otimes \mathbf{e}_i. \quad (3.39)$$

The limit as $\varepsilon \rightarrow 0$ in (3.25) with test function $\varphi(\mathbf{x}, t)$, vanishing at the boundaries S^+ and S^- , and at $t = 0$ and $t = T$ results in the macroscopic continuity equation:

$$\begin{aligned} 0 &= \int_{\Omega_T} \left((\chi^\varepsilon \rho_f + (1 - \chi^\varepsilon) \rho_s) \frac{\partial \varphi}{\partial t} + \rho_f \mathbf{v}^\varepsilon \cdot \nabla \varphi \right) dx dt \\ &= \int_{\Omega_T} \left((\chi(\mathbf{x}, t, \frac{\mathbf{x}}{\varepsilon}) \rho_f + (1 - \chi(\mathbf{x}, t, \frac{\mathbf{x}}{\varepsilon})) \rho_s) \frac{\partial \varphi}{\partial t} + \rho_f \mathbf{V}(\mathbf{x}, t, \frac{\mathbf{x}}{\varepsilon}) \cdot \nabla \varphi \right) dx dt + o(\varepsilon) \\ &\rightarrow \int_{\Omega_T} \left(m(\mathbf{x}, t) (\rho_f - \rho_s) + \rho_s \right) \frac{\partial \varphi}{\partial t} + \rho_f \mathbf{v}(\mathbf{x}, t) \cdot \nabla \varphi \, dx dt = 0, \end{aligned}$$

where $m(\mathbf{x}, t) = \int_Y \chi(\mathbf{x}, t, \mathbf{y}) d\mathbf{y}$ is the porosity of the pore space $\Omega^f(t)$.

Due to the arbitrary choice of $\varphi(\mathbf{x}, t)$ the latter identity is equivalent to the desired differential equation

$$\frac{\partial m}{\partial t} = \frac{\rho_f}{\rho_s - \rho_f} \nabla \cdot \mathbf{v} \quad (3.40)$$

in the domain Ω_T .

As before, we simply pass to the limit as $\varepsilon \rightarrow 0$ in the corresponding integral identity (3.26) for the acid concentration with arbitrary smooth functions $\xi(\mathbf{x}, t)$, vanishing at $t = T$ and at boundaries of S^\pm :

$$\begin{aligned} - \int_{\Omega} \chi_0(\mathbf{x}) \left(c_0(\mathbf{x}) + \frac{1}{\gamma} \right) \xi_0(\mathbf{x}, 0) dx &= \int_{\Omega_T} \chi^\varepsilon \left((c^\varepsilon + \frac{1}{\gamma}) \frac{\partial \xi}{\partial t} - (\alpha_c \nabla c^\varepsilon - \mathbf{v}^\varepsilon c^\varepsilon) \cdot \nabla \xi \right) dx dt \\ &= \int_{\Omega_T} \chi(\mathbf{x}, t, \frac{\mathbf{x}}{\varepsilon}) \left((c + \beta) \frac{\partial \xi}{\partial t} - \alpha_c (\nabla c + \nabla_y C(\mathbf{x}, t, \frac{\mathbf{x}}{\varepsilon})) - c \mathbf{V}(\mathbf{x}, t, \frac{\mathbf{x}}{\varepsilon}) \cdot \nabla \xi \right) dx dt + o(\varepsilon) \\ &\rightarrow \int_{\Omega_T} m(\mathbf{x}, t) \left((c + \frac{1}{\gamma}) \frac{\partial \xi}{\partial t} - (\alpha_c \mathbb{A} \cdot \nabla c - c \mathbf{v}) \cdot \nabla \xi \right) dx dt. \end{aligned}$$

Thus, $\frac{\partial}{\partial t} (m(c + \frac{1}{\gamma})) = \nabla \cdot (\alpha_c \mathbb{A} \cdot \nabla c - c \mathbf{v})$, where

$$\mathbb{A}(\mathbf{x}, t) = m(\mathbf{x}, t) \mathbb{I} + \sum_{i=1}^3 \langle \nabla_y C^{(i)}(\mathbf{x}, t, \mathbf{y}) \rangle_{Y_f} \otimes \mathbf{e}_i. \quad (3.41)$$

Functions $C^{(i)}(\mathbf{x}, t, \mathbf{y})$ are defined as solutions to the periodic boundary-value problem (see [22])

$$\nabla_y \cdot \left(\chi(\mathbf{x}, t, \mathbf{y}) (\nabla_y C^{(i)}(\mathbf{x}, t, \mathbf{y}) + \mathbf{e}_i) \right) = 0, \quad \mathbf{y} \in Y. \quad (3.42)$$

To get macroscopic transport equations for the concentrations of products of chemical reactions, we use representations (3.30) and pass to the limit as $\varepsilon \rightarrow 0$ in the corresponding integral identities

for the concentrations of products of chemical reactions

$$I_i^\varepsilon \equiv \int_{\Omega_T} \chi^\varepsilon \left(c_i^\varepsilon \frac{\partial \psi}{\partial t} + \left(c_i^\varepsilon - \frac{\rho_s c_i^0}{\rho_s - \rho_f} \right) \mathbf{v}^\varepsilon \cdot \nabla \psi \right) dxdt = 0, \quad i = 1, \dots, n,$$

which are valid for arbitrary smooth functions ψ , vanishing at the boundary S^- , and $t = T$.

One has

$$\begin{aligned} I_i^\varepsilon &= \int_{\Omega_T} \left(c_i \chi(\mathbf{x}, t, \frac{\mathbf{x}}{\varepsilon}) \frac{\partial \psi}{\partial t} + \left(c_i - \frac{\rho_s c_i^0}{\rho_s - \rho_f} \right) \mathbf{V}(\mathbf{x}, t, \frac{\mathbf{x}}{\varepsilon}) \cdot \nabla \psi \right) dxdt + o(\varepsilon) \\ &\rightarrow \int_{\Omega_T} \left(m c_i \frac{\partial \psi}{\partial t} + \left(c_i - \frac{\rho_s c_i^0}{\rho_s - \rho_f} \right) \mathbf{v} \cdot \nabla \psi \right) dxdt = 0. \end{aligned}$$

Therefore,

$$\int_{\Omega_T} \psi \left(\frac{\partial}{\partial t} (m c_i) + \nabla \cdot \left(\left(c_i - \frac{\rho_s c_i^0}{\rho_s - \rho_f} \right) \mathbf{v} \right) \right) dxdt = 0,$$

or $\frac{\partial}{\partial t} (m c_i) + \nabla \cdot \left(\left(c_i - \frac{\rho_s c_i^0}{\rho_s - \rho_f} \right) \mathbf{v} \right) = 0$. Using continuity equation (3.40) we arrive at the following transport equations $m \frac{\partial c_i}{\partial t} + \mathbf{v} \cdot \nabla c_i = \frac{\rho_s}{\rho_f} (c_i - c_i^0)$ for the concentrations of product of chemical reactions c_i for $i = 1, \dots, n$ in the domain Ω_T .

3.3.1. Initial-boundary value problem, describing in-situ leaching at the macroscopic level. Gathering all this together we get the final system of differential equations, describing the physical process in consideration at the macroscopic level.

This system consists of *Darcy's law*

$$\mathbf{v} = -\frac{1}{\mu_1} \mathbb{B}(\nabla q + \mathbf{f}) \quad (3.43)$$

and *the nonhomogeneous continuity equation*

$$\nabla \cdot \mathbf{v} = \delta \frac{\partial m}{\partial t}, \quad \delta = \frac{\rho_s - \rho_f}{\rho_f}, \quad (3.44)$$

for the velocity and pressure of the liquid, the *diffusion-convection equation*

$$\frac{\partial}{\partial t} \left(m \left(c + \frac{1}{\gamma} \right) \right) = \nabla \cdot (\alpha_c \mathbb{A} \cdot \nabla c - c \mathbf{v}) \quad (3.45)$$

for the acid, and *transport equations*

$$m \frac{\partial c_i}{\partial t} + \mathbf{v} \cdot \nabla c_i = \frac{\rho_s}{\rho_f} (c_i - c_i^0) \quad (3.46)$$

for the concentrations of the products of chemical reactions c_i , $i = 1, \dots, n$, in the domain Ω_T .

The problem is completed with the following boundary and initial conditions.

At the pumping wells $S^+ \subset \partial\Omega$ for $0 < t < T$ the pressure of the liquid and concentrations of the acid and products of chemical reactions are known functions

$$p = p^+(\mathbf{x}, t), \quad (3.47)$$

$$c_i = 0, \quad i = 1, \dots, n, \quad c = c^+(\mathbf{x}, t). \quad (3.48)$$

At the production wells $S^- \subset \partial\Omega$ for $0 < t < T$

$$p = p^-(\mathbf{x}, t), \quad (3.49)$$

$$c = c^+(\mathbf{x}, t). \quad (3.50)$$

At the impermeable boundary $S^0 \subset \partial\Omega$ for $0 < t < T$

$$\nabla c \cdot \mathbf{n} = 0, \quad (3.51)$$

$$\mathbf{v} \cdot \mathbf{n} = 0. \quad (3.52)$$

Matrix \mathbb{B} in (3.43) is defined in (3.34)–(3.37), (3.39), and matrix \mathbb{A} is defined in (3.41)–(3.42).

In turn, definitions of m , \mathbb{B} and \mathbb{A} contain the function $\chi(\mathbf{x}, t, \mathbf{y})$, its behavior for $0 < t < T$ is governed by the equation

$$\frac{\partial \chi}{\partial t} + \beta \gamma c(\mathbf{x}, t) |\nabla_{\mathbf{y}} \chi| = 0 \quad (3.53)$$

in the domain Y .

At the initial time

$$c(\mathbf{x}, 0) = c_0(\mathbf{x}), \quad c_i(\mathbf{x}, 0) = 0, \quad \mathbf{x} \in \Omega, \quad i = 1, \dots, n, \quad (3.54)$$

$$\chi(\mathbf{x}, 0, \mathbf{y}) = \chi_0(\mathbf{x}, \mathbf{y}), \quad \mathbf{x} \in \Omega, \quad \mathbf{y} \in Y. \quad (3.55)$$

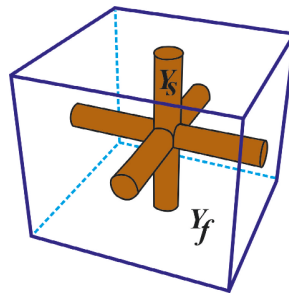


Fig. 3.12. The structure of the pore space

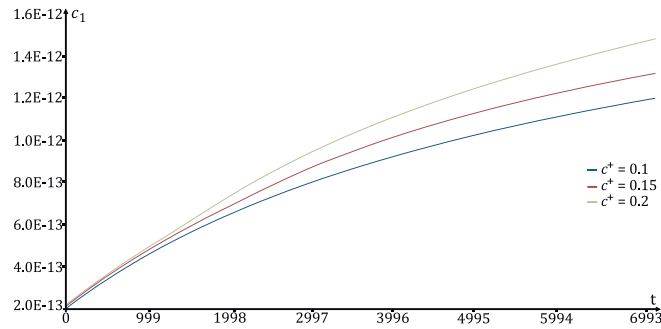


Fig. 3.13. The macroscopic model: concentration of product of chemical reaction at the pumping wells for different c^+

3.3.2. Numerical implementations. For the case of one spatial variable, let the pore space be defined by symmetric cylinders of radius r (see Fig. 3.12), $\Omega = \{0 < x < 1\}$, $S^+ = \{x = 0\}$, and $S^- = \{x = 1\}$. The symmetry of the pore space Y_f implies the diagonal form of matrices \mathbb{A} and \mathbb{D} : $\mathbb{A} = \text{diag}(k)$, $\mathbb{D} = \text{diag}(D_0)$. These values k and D_0 almost do not change for small variations of m and we may assume that they are constants. Under these assumptions the porosity m of the pore space is a known function of the radius r : $m = F(r) = 1 - (1 - m_0)(\frac{r}{r_0})^2$, where m_0 and r_0 are given initial values of the porosity m and radius r , the system (3.43)–(3.55) takes the form:

$$v = -\frac{k}{\mu_1} \frac{\partial p}{\partial x},$$

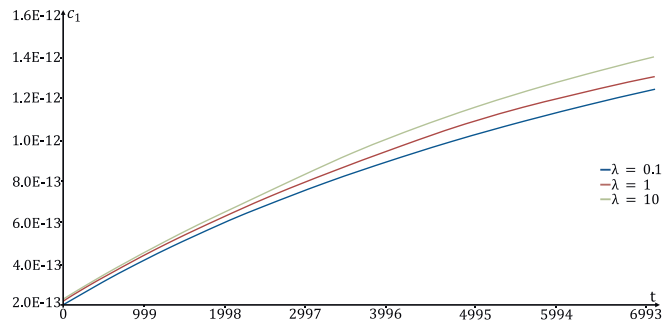


Fig. 3.14. The macroscopic model: concentration of product of chemical reaction at the pumping wells for different λ

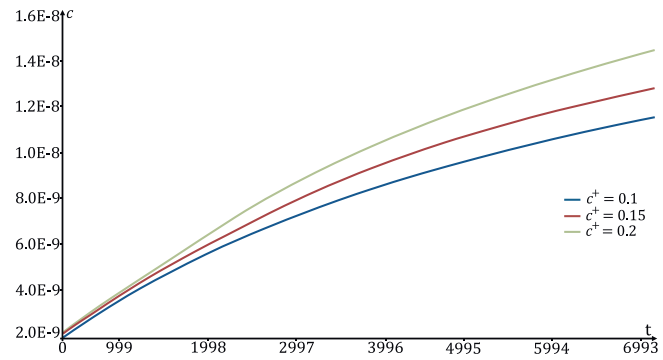


Fig. 3.15. The macroscopic model: concentration of the acid at the pumping wells for different c^+

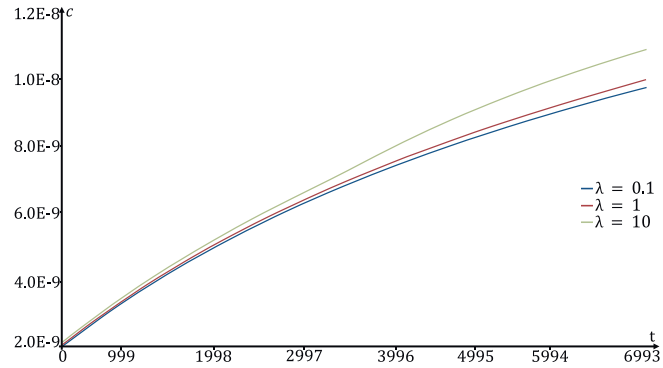


Fig. 3.16. The macroscopic model: concentration of the acid at the pumping wells for different λ

for k and μ_1 as constant values,

$$\begin{aligned} \frac{\partial v}{\partial x} &= \delta \frac{\partial m}{\partial t}, \\ \frac{\partial}{\partial t} \left(m \left(c + \frac{1}{\gamma} \right) \right) &= \frac{\partial}{\partial x} \left(\alpha_c \frac{\partial c}{\partial x} - v c \right), \\ m \frac{\partial c_i}{\partial t} + v \frac{\partial c_i}{\partial x} &= - \left(\delta (c_i - c_i^0) + c_i \right) \frac{\partial m}{\partial t}, \\ \frac{\partial r}{\partial t} &= \lambda c(x, t), \end{aligned}$$

$$\begin{aligned}
p(0,t) &= p^+(t), \quad p(1,t) = p^-(t), \quad t > 0, \\
c_i(0,t) &= 0, \quad i = 1, \dots, n, \quad c(0,t) = c^+(t), \quad \frac{\partial c}{\partial x}(1,t) = 0, \\
\begin{cases} c(x,0) = c_0(x), & c_i(x,0) = 0, \quad i = 1, \dots, n, \quad r(x,0) = r_0(x), \\ m(x,0) = m_0(x) \approx \pi r_0^2(x) + 2(r_0^2(x) - 2\pi r_0^3(x)). \end{cases}
\end{aligned}$$

For $\delta = 1.5$, $\gamma = 1$, $c_1^0 = 0.001$, $\alpha_c = 0.0004$, $T = 6993 \text{ sec}$, $p^+ = 1000$, $p^- = 0$, $c_0 = 0$, $r_0 = 2^{-1}$ we calculate concentration c_1 of the first product of chemical reactions at the pumping wells for different values of $c^+ = 0.1; 0.15; 0.2$ with fixed $\lambda = 1$, and for different values of $\lambda = 0.1; 1; 10$ with fixed $c^+ = 0.2$ (see Figs. 3.13–3.16).

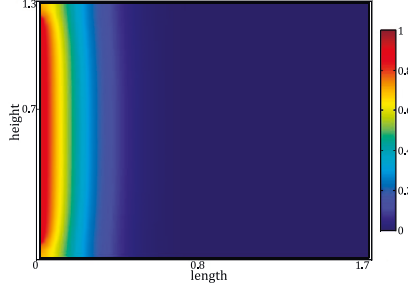


Fig. 3.17. The concentration of the reagent at t=360 days

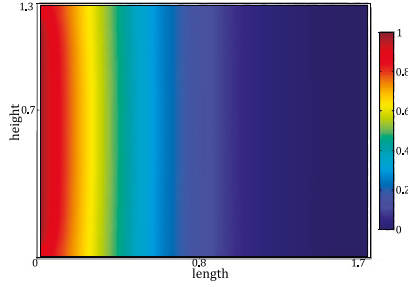


Fig. 3.18. The concentration of the reagent at t=720 days

For the case of two spacial variables and the system of differential equations in the domain $\Omega = \{0 < x_1 < L, 0 < x_2 < H\}$ (see Fig. 3.7) we have studied the initial-boundary value problem, describing in-situ leaching at the macroscopic level (3.43)–(3.55) and for $\delta = 1.5$, $\gamma = 1$, $c_1^0 = 0.01$, $\alpha_c = 0.004$, $p^+ = 1000$, $p^- = 0$, $c_0 = 0$ we have calculated concentration c_1 of the first product of chemical reactions at the pumping wells for different moments of time with fixed $c^+ = 1$ (see Fig. 3.17-3.18).

4. Dynamics of Cracks in Underground Rocks

4.1. Accumulation of the energy in a single crack: the microscopic (pore) level. Let Ω^0 be a bounded domain with a C^2 continuous boundary $S = \partial\Omega^0$ and $\Omega = \mathbb{R}^3 \setminus \overline{\Omega^0}$. We suppose that Ω is a poroelastic medium, which consists of the solid skeleton Ω^s and pore space Ω^f , and Ω^0 is a single crack. The crack Ω^0 and pore space Ω^f are filled by the same liquid.

In dimensionless variables $\mathbf{x} \rightarrow \frac{\mathbf{x}}{L}$, $\mathbf{w} \rightarrow \frac{\mathbf{w}}{L}$, $t \rightarrow \frac{t}{\tau}$, $\rho \rightarrow \frac{\rho}{\rho_0}$, the evolution of the displacements \mathbf{w} , pressure p , and temperature ϑ of the solid skeleton is governed in Ω^s for $t > 0$ by the nonisothermal Lamé equations [22]

$$\alpha_\tau \varrho_s \frac{\partial^2 \mathbf{w}}{\partial t^2} = \nabla \cdot \mathbb{P}_s, \tag{4.1}$$

$$\alpha_{p,s} \frac{\partial p}{\partial t} + \nabla \cdot \frac{\partial \mathbf{w}}{\partial t} = 0, \quad (4.2)$$

$$\frac{\partial \vartheta}{\partial t} = \Delta \vartheta. \quad (4.3)$$

The velocity $\mathbf{v} = \frac{\partial \mathbf{w}}{\partial t}$, pressure p , and temperature ϑ of the liquid satisfy in Ω^f and Ω^0 for $t > 0$ the Stokes system for a viscous compressible thermofluid

$$\alpha_{\tau} \varrho_f \frac{\partial^2 \mathbf{w}}{\partial t^2} = \nabla \cdot \mathbb{P}_f, \quad (4.4)$$

$$\alpha_{p,f} \frac{\partial p}{\partial t} + \nabla \cdot \frac{\partial \mathbf{w}}{\partial t} = 0, \quad (4.5)$$

$$\frac{\partial \vartheta}{\partial t} = \Delta \vartheta. \quad (4.6)$$

On the boundaries $S_f = \partial\Omega^s \cap \partial\Omega^0 \subset S$ and $\Gamma = \partial\Omega^s \cap \partial\Omega^f$ between Ω^s and Ω^0 , and between Ω^s and Ω^f correspondingly, displacements (velocities), normal tensions, temperature, and heat fluxes are continuous:

$$\lim_{\substack{\mathbf{x} \rightarrow \mathbf{x}^0 \in S_f \\ \mathbf{x} \in \Omega^s}} \mathbf{w}(\mathbf{x}, t) = \lim_{\substack{\mathbf{x} \rightarrow \mathbf{x}^0 \in S_f \\ \mathbf{x} \in \Omega^0}} \mathbf{w}(\mathbf{x}, t), \quad \lim_{\substack{\mathbf{x} \rightarrow \mathbf{x}^0 \in S_f \\ \mathbf{x} \in \Omega^s}} \vartheta(\mathbf{x}, t) = \lim_{\substack{\mathbf{x} \rightarrow \mathbf{x}^0 \in S_f \\ \mathbf{x} \in \Omega^0}} \vartheta(\mathbf{x}, t), \quad (4.7)$$

$$\lim_{\substack{\mathbf{x} \rightarrow \mathbf{x}^0 \in S_f \\ \mathbf{x} \in \Omega^s}} \mathbb{P}_s(\mathbf{x}, t) \cdot \mathbf{n} = \lim_{\substack{\mathbf{x} \rightarrow \mathbf{x}^0 \in S_f \\ \mathbf{x} \in \Omega^0}} \mathbb{P}_f(\mathbf{x}, t) \cdot \mathbf{n}, \quad \lim_{\substack{\mathbf{x} \rightarrow \mathbf{x}^0 \in S_f \\ \mathbf{x} \in \Omega^s}} \frac{\partial \vartheta}{\partial n}(\mathbf{x}, t) = \lim_{\substack{\mathbf{x} \rightarrow \mathbf{x}^0 \in S_f \\ \mathbf{x} \in \Omega^0}} \frac{\partial \vartheta}{\partial n}(\mathbf{x}, t), \quad (4.8)$$

$$\lim_{\substack{\mathbf{x} \rightarrow \mathbf{x}^0 \in \Gamma \\ \mathbf{x} \in \Omega^s}} \mathbf{w}(\mathbf{x}, t) = \lim_{\substack{\mathbf{x} \rightarrow \mathbf{x}^0 \in \Gamma \\ \mathbf{x} \in \Omega^f}} \mathbf{w}(\mathbf{x}, t), \quad \lim_{\substack{\mathbf{x} \rightarrow \mathbf{x}^0 \in \Gamma \\ \mathbf{x} \in \Omega^s}} \vartheta(\mathbf{x}, t) = \lim_{\substack{\mathbf{x} \rightarrow \mathbf{x}^0 \in \Gamma \\ \mathbf{x} \in \Omega^f}} \vartheta(\mathbf{x}, t), \quad (4.9)$$

$$\lim_{\substack{\mathbf{x} \rightarrow \mathbf{x}^0 \in \Gamma \\ \mathbf{x} \in \Omega^s}} \mathbb{P}_s(\mathbf{x}, t) \cdot \mathbf{n} = \lim_{\substack{\mathbf{x} \rightarrow \mathbf{x}^0 \in \Gamma \\ \mathbf{x} \in \Omega^f}} \mathbb{P}_f(\mathbf{x}, t) \cdot \mathbf{n}, \quad \lim_{\substack{\mathbf{x} \rightarrow \mathbf{x}^0 \in \Gamma \\ \mathbf{x} \in \Omega^s}} \frac{\partial \vartheta}{\partial n}(\mathbf{x}, t) = \lim_{\substack{\mathbf{x} \rightarrow \mathbf{x}^0 \in \Gamma \\ \mathbf{x} \in \Omega^f}} \frac{\partial \vartheta}{\partial n}(\mathbf{x}, t). \quad (4.10)$$

The surface $S \setminus S_f$ is the boundary between the liquid in Ω^f and the liquid in Ω^0 , and we do not need any boundary condition there because it is the same liquid.

The problem is completed with initial conditions

$$\mathbf{w}(\mathbf{x}, 0) = \frac{\partial \mathbf{w}}{\partial t}(\mathbf{x}, 0) = 0, \quad \mathbf{x} \in \mathbb{R}^3, \quad (4.11)$$

$$\vartheta(\mathbf{x}, 0) = \vartheta^0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3. \quad (4.12)$$

In (4.7)–(4.10) \mathbf{n} is a normal vector to the boundary Γ , $\mathbb{P}_f = \alpha_{\mu} \mathbb{D}(x, \mathbf{v}) - (p + \alpha \vartheta) \mathbb{I}$, $\mathbb{P}_s = \alpha_{\lambda} \mathbb{D}(x, \mathbf{w}) - (p + \alpha \vartheta) \mathbb{I}$, $\mathbb{D}(x, \mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^*)$, $\alpha_{\tau} = \frac{L}{g\tau^2}$, $\alpha_{\mu} = \frac{2\mu}{\tau L g \rho^0}$, $\alpha_{\lambda} = \frac{2\lambda}{L g \rho^0}$, $\alpha_{p,f} = \frac{L g}{\varrho_f c_f^2}$, $\alpha_{p,s} = \frac{L g}{\varrho_s c_s^2}$, L is the characteristic size of the physical domain in consideration, τ is the characteristic time of the physical process, ρ^0 is the mean density of water, g is the acceleration due to gravity, ϱ_f and ϱ_s are the respective mean dimensionless densities of the liquid in pores and the solid skeleton, correlated with the mean density of water ρ^0 , $\mu = \text{const}$ is the viscosity of the liquid, $\lambda = \text{const}$ is the Lamé's coefficient of the solid skeleton, and \mathbb{I} is the unit tensor. Positive constants c_f and c_s are the speed of compressive sound waves in the pore liquid and in the solid skeleton respectively [22].

Function ϑ_0 is infinitely smooth

$$\vartheta_0 \in C^{\infty}(\mathbb{R}^3) \quad (4.13)$$

and has a finite support.

Dimensionless criteria α_{τ} , α_{μ} , α_{λ} are different for different physical processes. Some of them might be small, some of them might be large. Accumulation in time of the energy in cracks is a long-term process. Therefore α_{τ} and α_{μ} are sufficiently small, while α_{λ} is close to unity.

It is clear that the mathematical model of a physical process should be as simple as possible, but must still describe all of its main features. That is why we use homogenization to simplify exact

mathematical models at the pore scale. Note that any additional term in a mathematical model at the pore scale creates additional technical problems in the homogenization. Therefore, we should do all simplifications before homogenization.

For joint motion of the elastic skeleton and liquid in pores when the velocity of acoustic waves is so great that they do not play any significant role, one usually neglects the inertial term $\alpha_\tau \frac{\partial^2 \mathbf{w}}{\partial t^2}$ in dynamic equation (4.1) for the elastic skeleton:

$$\nabla \cdot \mathbb{P}_s = 0, \quad \mathbf{x} \in \Omega^s, \quad t > 0. \quad (4.14)$$

The second significant simplification is the assumption that

$$\alpha_\mu = \mu \varepsilon^2, \quad (4.15)$$

where $\varepsilon = \frac{l}{L}$ is the dimensionless pore size and l is the average size of pores.

This assumption for the stationary Stokes system results in the well-known Darcy's law for liquid motion in the pores of an absolutely rigid body.

But if we consider a joint motion of the viscous compressible liquid in pores and in a reservoir governed by the stationary Stokes system under this assumption, then after homogenization we arrive at the system of differential equations

$$\nabla p + \mathbf{f} = 0, \quad \alpha_{p,f} \frac{\partial p}{\partial t} + \nabla \cdot \mathbf{v} = 0$$

in the reservoir, which does not determine the motion inside the crack.

Thus, combining the nonstationary Lamé's equations and the Stokes system (4.1) and (4.4) is the best method to describe the joint motion of the elastic skeleton, the liquid in pores and the liquid in the crack.

To estimate displacements, we multiply equation (4.1) by $\frac{\partial \mathbf{w}}{\partial t}$ and integrate the result of multiplication over the domain Ω^s . Next we multiply equation (4.4) by $\frac{\partial \mathbf{w}}{\partial t}$ and integrate the result of multiplication over the domains Ω^f and Ω^0 and sum the integrals, obtaining the following expressions after integration by parts:

$$\begin{aligned} & \frac{\alpha_\tau}{2} \frac{d}{dt} \int_{\mathbb{R}^3} \left(((1 - \chi_0)\chi + \chi_0)\varrho_f + (1 - \chi)\varrho_s \right) \left| \frac{\partial \mathbf{w}}{\partial t}(\mathbf{x}, t) \right|^2 dx \\ & + \frac{\alpha_\lambda}{2} \frac{d}{dt} \int_{\mathbb{R}^3} (1 - \chi_0)(1 - \chi) \mathbb{D}(x, \mathbf{w}(\mathbf{x}, t)) : \mathbb{D}(x, \mathbf{w}(\mathbf{x}, t)) dx \\ & + \alpha_\mu \int_{\mathbb{R}^3} \left((1 - \chi_0)\chi^\varepsilon + \chi_0 \right) \mathbb{D}\left(x, \frac{\partial \mathbf{w}}{\partial t}(\mathbf{x}, t)\right) : \mathbb{D}\left(x, \frac{\partial \mathbf{w}}{\partial t}(\mathbf{x}, t)\right) dx \\ & - \int_{\Omega^s} p(\mathbf{x}, t) \nabla \cdot \frac{\partial \mathbf{w}}{\partial t}(\mathbf{x}, t) dx - \int_{\Omega^f \cup \Omega^0} p(\mathbf{x}, t) \nabla \cdot \frac{\partial \mathbf{w}}{\partial t}(\mathbf{x}, t) dx = \alpha \int_{\mathbb{R}^3} \vartheta(\mathbf{x}, t) \nabla \cdot \frac{\partial \mathbf{w}}{\partial t}(\mathbf{x}, t) dx. \end{aligned}$$

Integrals over the boundary Γ disappear due to boundary conditions (4.7)–(4.10).

In the sequel, we exclude $\nabla \cdot \frac{\partial \mathbf{w}}{\partial t}$ in the last three terms using equations (4.2) and (4.5), and integrate the result with respect to time over the interval $(0, T)$

$$\frac{\alpha_\tau}{2} \int_{\mathbb{R}^3} (\chi \varrho_f + (1 - \chi)\varrho_s) \frac{\partial \mathbf{w}}{\partial t}(\mathbf{x}, t) \cdot \frac{\partial \mathbf{w}}{\partial t}(\mathbf{x}, t) dx + \frac{\alpha_{p,s}}{4} \int_{\Omega^s} |p(\mathbf{x}, t)|^2 dx + \frac{\alpha_{p,f}}{4} \int_{\Omega^f \cup \Omega^0} |p(\mathbf{x}, t)|^2 dx$$

$$\begin{aligned}
& + \frac{1}{4\alpha_{p,s}} \int_{\Omega^s} |\nabla \cdot \mathbf{w}(\mathbf{x}, t)|^2 dx + \frac{1}{4\alpha_{p,f}} \int_{\Omega^f \cup \Omega^0} |\nabla \cdot \mathbf{w}(\mathbf{x}, t)|^2 dx + \frac{\alpha_\lambda}{2} \int_{\Omega^s} \mathbb{D}(x, \mathbf{w}(\mathbf{x}, t)) : \mathbb{D}(x, \mathbf{w}(\mathbf{x}, t)) dx \\
& + \alpha_\mu \int_0^T \int_{\Omega^f \cup \Omega^0} \mathbb{D}(x, \frac{\partial \mathbf{w}}{\partial t}(\mathbf{x}, t)) : \mathbb{D}(x, \frac{\partial \mathbf{w}}{\partial t}(\mathbf{x}, t)) dx dt \\
& = \alpha \int_{\mathbb{R}^3} \vartheta(\mathbf{x}, t) \nabla \cdot \mathbf{w}(\mathbf{x}, t) dx - \alpha \int_0^T \int_{\mathbb{R}^3} \frac{\partial \vartheta}{\partial t}(\mathbf{x}, t) \nabla \cdot \mathbf{w}(\mathbf{x}, t) dx dt. \quad (4.16)
\end{aligned}$$

The temperature ϑ and its time derivative $\frac{\partial \vartheta}{\partial t}$ are bounded and tend to zero as $t \rightarrow \infty$. It follows from the equations and boundary conditions, and from [17] that we have

$$\vartheta(\mathbf{x}, t) = \frac{1}{(4\pi t)^{\frac{3}{2}}} \int_{\mathbb{R}^3} \exp\left(-\frac{|\mathbf{x} - \mathbf{y}|}{4t}\right) \vartheta_0(\mathbf{y}) dy \quad (4.17)$$

and (4.13).

Thus,

$$\begin{aligned}
& \max_{0 < t < \infty} \left(\alpha_\tau \int_{\mathbb{R}^3} \left| \frac{\partial \mathbf{w}}{\partial t}(\mathbf{x}, t) \right|^2 dx + \int_{\Omega^s} \mathbb{D}(x, \mathbf{w}(\mathbf{x}, t)) : \mathbb{D}(x, \mathbf{w}(\mathbf{x}, t)) dx \right) \\
& + \max_{0 < t < \infty} \int_{\mathbb{R}^3} |p(\mathbf{x}, t)|^2 dx + \max_{0 < t < \infty} \int_{\mathbb{R}^3} |\nabla \cdot \mathbf{w}(\mathbf{x}, t)|^2 dx \\
& + \alpha_\mu \int_0^\infty \int_{\Omega^f \cup \Omega^0} \mathbb{D}(x, \frac{\partial \mathbf{w}}{\partial t}(\mathbf{x}, t)) : \mathbb{D}(x, \frac{\partial \mathbf{w}}{\partial t}(\mathbf{x}, t)) dx dt \leq C,
\end{aligned}$$

where C depend only on the norms on the interval $[0, \infty)$ of ϑ and $\frac{\partial \vartheta}{\partial t}$ given by (4.17).

Let χ_0 be the characteristic function of the domain Ω^0 , and χ be the characteristic function of the domain Ω^f : $\chi_0(\mathbf{x}) = 1$ for $\mathbf{x} \in \Omega^0$ and $\chi_0(\mathbf{x}) = 0$ for $\mathbf{x} \in \mathbb{R}^3 \setminus \Omega^0$, $\chi(\mathbf{x}) = 1$ for $\mathbf{x} \in \Omega^f$ and $\chi(\mathbf{x}) = 0$ for $\mathbf{x} \in \Omega^s$.

The latter estimate shows that the problem (4.1)–(4.5), (4.7), (4.8), (4.12)–(4.14) has a unique weak solution in the sense of distributions: functions \mathbf{w} , p , and ϑ satisfy integral identity

$$\begin{aligned}
& - \alpha_\tau \int_0^T \int_{\mathbb{R}^3} \left(\varrho_f(\chi^0 + (1 - \chi^0)\chi) + \varrho_s(1 - \chi^0)(1 - \chi) \right) \frac{\partial \mathbf{w}}{\partial t} \cdot \frac{\partial \varphi}{\partial t} dx dt \\
& + \int_0^T \int_{\mathbb{R}^3} \left((1 - \chi_0)(\chi \mathbb{P}_f + (1 - \chi)\mathbb{P}_s) + \chi_0 \mathbb{P}_f \right) : \mathbb{D}(x, \varphi) dx dt = 0 \quad (4.18)
\end{aligned}$$

for any smooth functions φ with compact support, and the continuity equation

$$(\chi \alpha_{p,f} + (1 - \chi) \alpha_{p,s}) p + \nabla \cdot \mathbf{w} = 0 \quad (4.19)$$

in the usual sense in \mathbb{R}^3 for any interval $0 < t < T$.

Let

$$\begin{aligned} \Pi(\Omega, t) = & \int_{\mathbb{R}^3} \alpha_\lambda (1 - \chi_0) (1 - \chi) \mathbb{D}(x, \mathbf{w}(\mathbf{x}, t)) : \mathbb{D}(x, \mathbf{w}(\mathbf{x}, t)) dx \\ & + \int_{\mathbb{R}^3} \left(\alpha_{p,f} (\chi_0 + (1 - \chi_0) \chi) + (1 - \chi_0) (1 - \chi) \alpha_{p,s} \right) |p(\mathbf{x}, t)|^2 dx \end{aligned}$$

denote the potential energy of the domain Ω at time t , and as $\Pi(\Omega^0, t) = \int_{\mathbb{R}^3} \alpha_{p,f} \chi_0 |p(\mathbf{x}, t)|^2 dx$ we denote the potential energy of the crack Ω^0 at the same moment t .

At the at $t = 0$ $\Pi(\Omega, 0) = \Pi(\Omega^0, 0) = 0$. Only relations (4.16) show how potential energies $\Pi(\Omega, t)$ and $\Pi(\Omega^0, t)$ behave after the heat impact. Will they be positive? And if they are positive then will they preserve their strictly positive values as $T \rightarrow \infty$?

This means exactly the accumulation of the energy in the crack during the heat impact, if $\Pi(\Omega, t)$ and $\Pi(\Omega^0, t)$ preserve their strictly positive values as $T \rightarrow \infty$. But we cannot state exactly this fact because of the presence of viscous energy $I_\infty = \alpha_\mu \int_0^\infty \int_{\mathbb{R}^3} \mathbb{D}(x, \frac{\partial \mathbf{w}}{\partial t}(\mathbf{x}, t)) : \mathbb{D}(x, \frac{\partial \mathbf{w}}{\partial t}(\mathbf{x}, t)) dx dt$. This is certainly strictly positive and the other term on the right-hand side of (4.16) might be zero at infinity.

This is why we are going to analyze this situation for the homogenized system under the assumption $\alpha_\mu \rightarrow 0$ as $\varepsilon \rightarrow 0$.

4.2. Energy accumulation in a single crack: the macroscopic description. Let a pore space Ω^f be defined by the characteristic function $\chi^\varepsilon(\mathbf{x}) = \chi(\frac{\mathbf{x}}{\varepsilon})$ with 1-periodic in \mathbf{y} function $\chi(\mathbf{y})$, $\mathbf{y} \in Y$, $Y = (0, 1)^3 \in \mathbb{R}^3$, $Y_f = \{\mathbf{y} \in Y : \chi(\mathbf{y}) = 1\}$, $Y_s = \{\mathbf{y} \in Y : \chi(\mathbf{y}) = 0\}$. The boundary γ between Y_f and Y_s is supposed to be Lipschitz continuous.

We look for the homogenized system under the following assumptions: $\alpha_\mu = \mu_3 \varepsilon^3$, $\alpha_\tau = \tau_0$, $\alpha_\lambda = \lambda_3 \varepsilon^3$, where μ_3 , τ_0 , and λ_3 do not depend on ε .

Let for given $\varepsilon > 0$ functions \mathbf{w}^ε , p^ε , and ϑ^ε be a solution of problem (4.1)–(4.12). We suppose that

$$\begin{cases} \chi^0(\mathbf{x}) \mathbf{w}^\varepsilon(\mathbf{x}, t) = \chi^0(\mathbf{x}) \mathbf{w}_f(\mathbf{x}, t) + o(\varepsilon), \\ (1 - \chi^0(\mathbf{x})) \chi^\varepsilon(\mathbf{x}) \mathbf{w}^\varepsilon(\mathbf{x}, t) = (1 - \chi^0(\mathbf{x})) \chi^\varepsilon(\mathbf{x}) \mathbf{w}(\mathbf{x}, t) + o(\varepsilon), \\ (1 - \chi^0(\mathbf{x})) (1 - \chi^\varepsilon(\mathbf{x})) \mathbf{w}^\varepsilon(\mathbf{x}, t) = (1 - \chi^0(\mathbf{x})) (1 - \chi^\varepsilon(\mathbf{x})) \mathbf{w}(\mathbf{x}, t) + o(\varepsilon), \end{cases} \quad (4.20)$$

$$p^\varepsilon(\mathbf{x}, t) = \chi^0 p_f(\mathbf{x}, t) + (1 - \chi^0) p(\mathbf{x}, t) + o(\varepsilon). \quad (4.21)$$

To derive homogenized dynamic equations, we use representations (4.20)–(4.21) in the integral identity (4.18) and pass from there to the limit as $\varepsilon \rightarrow 0$

$$\begin{aligned} 0 = & \int_0^T \int_{\mathbb{R}^3} \alpha_\tau \left(\varrho_f ((1 - \chi_0) \chi^\varepsilon + \chi_0) + \varrho_s (1 - \chi^0) (1 - \chi^\varepsilon) \right) \frac{\partial \mathbf{w}^\varepsilon}{\partial t} \cdot \frac{\partial \varphi}{\partial t} dx dt \\ & + \int_0^T \int_{\mathbb{R}^3} (\chi^0 (p_f + \alpha \vartheta) + (1 - \chi^0) (p + \alpha \vartheta)) \nabla \cdot \varphi dx dt - \int_0^T \int_{\mathbb{R}^3} \alpha_\mu ((1 - \chi_0) \chi^\varepsilon + \chi_0) \mathbb{D}(x, \frac{\partial \mathbf{w}^\varepsilon}{\partial t}) : \mathbb{D}(x, \varphi) dx dt \\ & - \int_0^T \int_{\mathbb{R}^3} \alpha_\lambda (1 - \chi_0) (1 - \chi^\varepsilon) \mathbb{D}(x, \mathbf{w}^\varepsilon) : \mathbb{D}(x, \varphi) dx dt + o(\varepsilon) \rightarrow I, \end{aligned}$$

$$I = \int_0^T \int_{\mathbb{R}^3} \left(\tau_0 \varrho_f \frac{\partial \mathbf{w}_f}{\partial t} + \hat{\varrho} (1 - \chi_0) \frac{\partial \mathbf{w}}{\partial t} \right) \cdot \frac{\partial \varphi}{\partial t} + (\chi^0 (p_f + \alpha \vartheta) + (1 - \chi^0) (p + \alpha \vartheta)) \nabla \cdot \varphi dx dt = 0,$$

where $\hat{\varrho} = m \varrho_f + (1 - m) \varrho_s$.

To derive the macroscopic continuity equation, we consider a corresponding mass conservation law in a form of the integral identity at the microscopic level. To this end, we multiply equations (4.2) and (4.5) by a test function ξ with compact support, integrate by parts over corresponding domains and sum results

$$\int_0^T \int_{\mathbb{R}^3} \left((\alpha_{p,f} (\chi^0 p_f + (1 - \chi^0) \chi^\varepsilon p) + \alpha_{p,s} (1 - \chi^0) (1 - \chi^\varepsilon) p) \xi - (\chi^0 \mathbf{w}_f + (1 - \chi^0) \mathbf{w}) \cdot \nabla \xi \right) dx dt = o(\varepsilon).$$

After the limit as $\varepsilon \rightarrow 0$ we arrive at the integral identity

$$\int_0^T \int_{\mathbb{R}^3} \left((\alpha_{p,f} (\chi^0 p_f + (1 - \chi^0) m p) + \alpha_{p,s} (1 - \chi^0) (1 - m) p) \xi - (\chi^0 \mathbf{w}_f + (1 - \chi^0) \mathbf{w}) \cdot \nabla \xi \right) dx dt = 0,$$

which is equivalent to the macroscopic continuity equation

$$\hat{c}_p p + \nabla \cdot \mathbf{w} = 0$$

in Ω for $t > 0$ ($\chi^0 = 0$), where $\hat{c}_p = m \alpha_{p,f} + (1 - m) \alpha_{p,s}$, and the continuity equation

$$\alpha_{p,f} p_f + \nabla \cdot \mathbf{w}_f = 0$$

in Ω^0 for $t > 0$ ($\chi^0 = 1$).

4.2.1. A joint motion of the elastic body and the liquid in crack. This joint motion is described by the system of integral identities

$$\int_0^T \int_{\mathbb{R}^3} \left(\tau_0 (\varrho_f \chi^0 \frac{\partial \mathbf{w}_f}{\partial t} + \hat{\varrho} (1 - \chi^0) \frac{\partial \mathbf{w}}{\partial t}) \cdot \frac{\partial \varphi}{\partial t} + (\chi^0 (p_f + \alpha \vartheta) + (1 - \chi^0) (p + \alpha \vartheta)) \nabla \cdot \varphi \right) dx dt = 0, \quad (4.22)$$

$$\int_0^T \int_{\mathbb{R}^3} \left((\alpha_{p,f} (\chi^0 p_f + (1 - \chi^0) m p) + \alpha_{p,s} (1 - \chi^0) (1 - m) p) \xi - (\chi^0 \mathbf{w}_f + (1 - \chi^0) \mathbf{w}) \cdot \nabla \xi \right) dx dt = 0, \quad (4.23)$$

which are valid for all smooth functions φ and ξ with compact supports.

It contains dynamics and continuity equations

$$\tau_0 \hat{\varrho} \frac{\partial \mathbf{v}}{\partial t} + \nabla (p + \alpha \vartheta) = 0, \quad (4.24)$$

$$\hat{c}_p \frac{\partial p}{\partial t} + \nabla \cdot \mathbf{v} = 0 \quad (4.25)$$

for the velocity $\mathbf{v} = \frac{\partial \mathbf{w}}{\partial t}$ and pressures p of the poroelastic medium in the domain Ω for $t > 0$, and dynamics and continuity equations for the liquid velocity $\mathbf{v} = \frac{\partial \mathbf{w}_f}{\partial t}$ and pressure p_f

$$\tau_0 \varrho_f \frac{\partial \mathbf{v}_f}{\partial t} + \nabla (p_f + \alpha \vartheta) = 0, \quad (4.26)$$

$$\alpha_{p,f} \frac{\partial p_f}{\partial t} + \nabla \cdot \mathbf{v}_f = 0, \quad (4.27)$$

in the crack Ω^0 for $t > 0$, and boundary conditions

$$p = p_f, \quad (4.28)$$

$$\mathbf{v} \cdot \mathbf{n} = \mathbf{v}_f \cdot \mathbf{n} \quad (4.29)$$

at the boundary S , where \mathbf{n} is a unit normal to S .

The problem is completed with initial conditions

$$\mathbf{v}_f(\mathbf{x}, 0) = 0, \quad \mathbf{x} \in \Omega^0, \quad (4.30)$$

$$\mathbf{v}(\mathbf{x}, 0) = 0, \quad \mathbf{x} \in \Omega. \quad (4.31)$$

Note that in (4.22)–(4.31) the temperature ϑ is given by (4.17).

4.2.2. Accumulation of the energy in a single crack. To get the basic integral identity, we multiply equation (4.26) for the liquid velocity in the crack by \mathbf{v}_f and integrate by parts over the domain Ω^0 . Then we multiply equation (4.24) by the velocity \mathbf{v} of the poroelastic medium, integrate by parts over the domain Ω and sum the equalities obtained

$$\begin{aligned} & \frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^3} \left(\tau_0 (\varrho_f \chi_0 |\mathbf{v}_f(\mathbf{x}, t)|^2 + \hat{\varrho}(1-\chi_0) |\mathbf{v}(\mathbf{x}, t)|^2) + (\alpha_{p,f} \chi^0 |p_f(\mathbf{x}, t)|^2 + \hat{c}_p (1-\chi^0) |p(\mathbf{x}, t)|^2) \right) dx \\ &= \alpha \frac{d}{dt} \int_{\mathbb{R}^3} \vartheta (\alpha_{p,f} \chi^0 p_f(\mathbf{x}, t) + \hat{c}_p (1-\chi^0) p(\mathbf{x}, t)) dx - \alpha \int_{\mathbb{R}^3} \frac{\partial \vartheta}{\partial t} (\alpha_{p,f} \chi^0 p_f(\mathbf{x}, t) + \hat{c}_p (1-\chi^0) p(\mathbf{x}, t)) dx. \end{aligned}$$

Integration over $(0, T)$ gives us

$$\begin{aligned} & \frac{1}{2} \int_{\mathbb{R}^3} \left(\tau_0 (\varrho_f \chi_0 |\mathbf{v}_f(\mathbf{x}, T)|^2 + \hat{\varrho}(1-\chi_0) |\mathbf{v}(\mathbf{x}, T)|^2) + (\alpha_{p,f} \chi^0 |p_f(\mathbf{x}, T)|^2 + \hat{c}_p (1-\chi^0) |p(\mathbf{x}, T)|^2) \right) dx \\ &= \alpha \int_{\mathbb{R}^3} \vartheta(\mathbf{x}, T) (\alpha_{p,f} \chi^0 p_f(\mathbf{x}, T) + \hat{c}_p (1-\chi^0) p(\mathbf{x}, T)) dx \\ &\quad - \alpha \int_0^T \int_{\mathbb{R}^3} \frac{\partial \vartheta}{\partial t}(\mathbf{x}, t) (\alpha_{p,f} \chi^0 p_f(\mathbf{x}, t) + \hat{c}_p (1-\chi^0) p(\mathbf{x}, t)) dx dt. \quad (4.32) \end{aligned}$$

Representation (4.17) implies $\lim_{T \rightarrow \infty} \vartheta(\mathbf{x}, T) = \lim_{T \rightarrow \infty} \frac{\partial \vartheta}{\partial t}(\mathbf{x}, T) = 0$ and $\frac{\partial \vartheta}{\partial t}(\mathbf{x}, t) < 0$ for $t > 0$. Therefore,

$$\begin{aligned} & \alpha \int_{\mathbb{R}^3} \vartheta(\mathbf{x}, T) (\alpha_{p,f} \chi^0 p_f(\mathbf{x}, T) + \hat{c}_p (1-\chi^0) p(\mathbf{x}, T)) dx \rightarrow 0, \\ & -\alpha \int_0^T \int_{\mathbb{R}^3} \frac{\partial \vartheta}{\partial t}(\mathbf{x}, t) (\alpha_{p,f} \chi^0 p_f(\mathbf{x}, t) + \hat{c}_p (1-\chi^0) p(\mathbf{x}, t)) dx dt \rightarrow E^* > 0, \\ & \Pi(\Omega^0, T) = \int_{\mathbb{R}^3} \alpha_{p,f} \chi_0 |p_f(\mathbf{x}, T)|^2 dx \rightarrow \Pi^* > 0 = \Pi(\Omega^0, T) \end{aligned}$$

as $T \rightarrow \infty$. This is exactly the accumulation of the energy in the crack during the heat impact.

4.3. Macroscopic model of crack propagation. As we have shown before, the potential energy $\Pi(\Omega^0, T)$ is increasing in time. It is very natural to suppose that for every single crack there exists some limit $P_* = P_*(\Omega^0)$ for the average pressure $P(T) = P(\Omega^0; T) = \frac{1}{V(\Omega^0, t)} \int_{\Omega^0} |p_f(\mathbf{x}, T)| dx$ inside this geological fault Ω^0 such that at the moment t_* , when $P(\Omega^0, t_*) = P_*$, this fracture starts to collapse.

We will describe the motion of the fracture after this specific moment t_* by mean of the curvature flow [8]

$$D_n = \sigma (P_* - P) k, \quad (4.33)$$

where D_n is a velocity of the moving (free) boundary $S = \partial\Omega^0$ toward the outer normal \mathbf{n} to S and k is a mean curvature of S .

More precisely, this mechanism is governed by the hysteresis law (see Fig. 4.1).

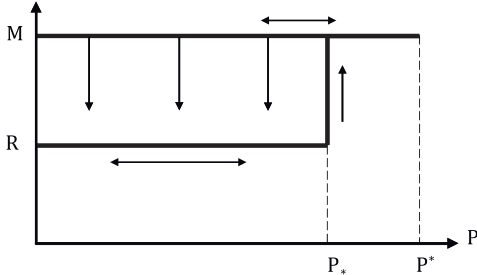


Fig. 4.1. Hysteresis law for the crack propagation

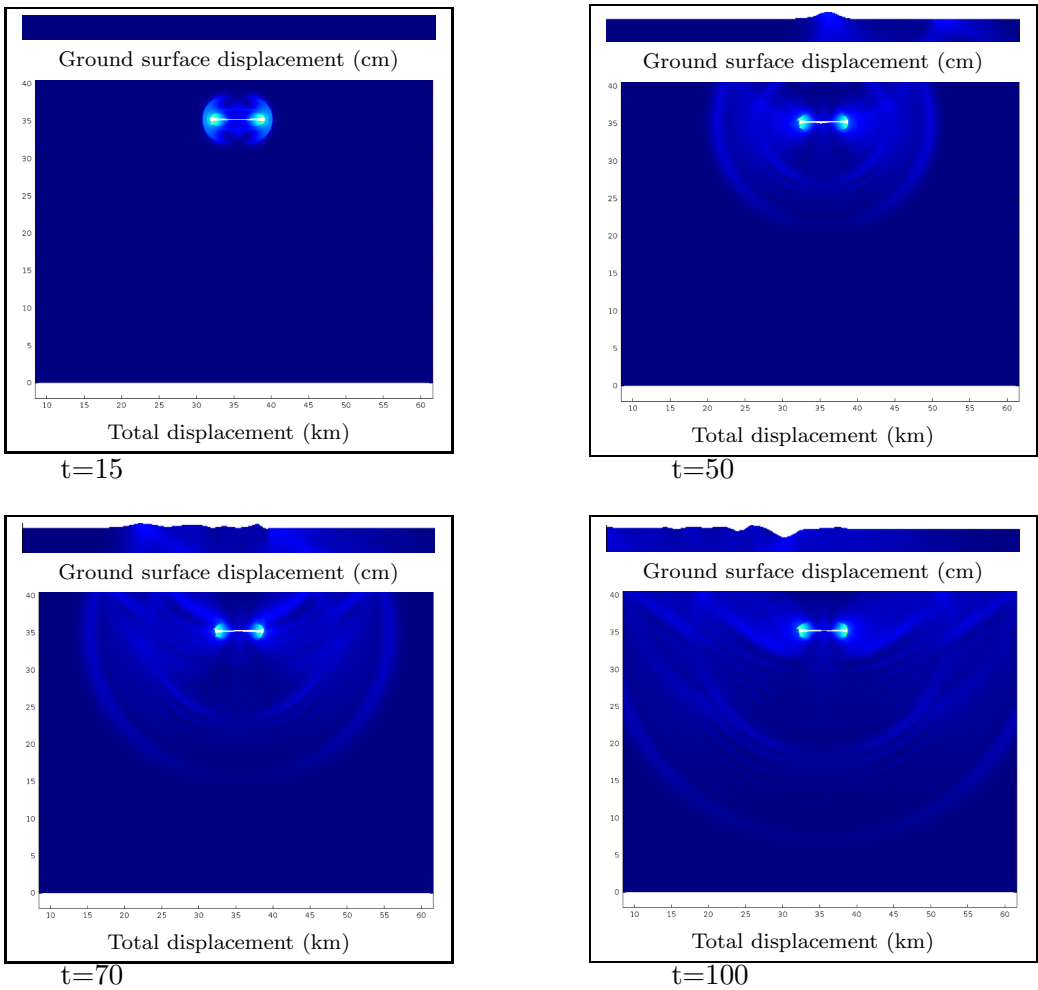


Fig. 4.2. Dynamics of a crack in rock

There are two positions for the state of the crack. The position **M** stands for the motion of the crack and the position **R** stands for the state of rest. If in the state of rest the average pressure P

achieves the limiting value P_* the crack changes state from \mathbf{R} to \mathbf{M} and starts to move. We assume that the product of average pressure and the volume V of crack are the same during the movement:

$$P(t) \cdot V(t) = \text{const.} \quad (4.34)$$

Thus, when the crack propagates and its volume decreases, the pressure $P(t)$ inside the crack increases up to value P_* and after that the crack returns to the position \mathbf{R} .

Obviously, the movement of the fracture creates seismic waves, which may reach the Earth's surface.

This stage of the process can be described by Lamé's system of elasticity

$$\alpha_{\tau} \rho_s \frac{\partial^2 \mathbf{w}}{\partial t^2} = \nabla \cdot (\alpha_{\lambda} \mathbb{D}(x, \mathbf{w}) - p \mathbb{I})$$

for the displacements \mathbf{w} and pressure p of the rock material in the domain Ω , coupled with the mean curvature flow (4.33) for the free boundary S of the domain Ω^0 . The problem is completed with the postulate (4.34), which gives boundary conditions

$$(\alpha_{\lambda} \mathbb{D}(x, \mathbf{w}) - p \mathbb{I}) \cdot \mathbf{n} = -P(t) \mathbf{n}$$

for the Lamé equations at the boundary S . Corresponding numerical implementations [24] confirm this suggested model (see Fig. 4.2).

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