

Numerical modeling of the liquid front propagation in inhomogeneous nanoporous media

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Abstract. In the last decade nanoporous materials applications in biology and medicine have been widely researched. One of the problems in this field are the transport processes in nanoporous media. The paper presents the numerical model, which simulates the motion of front of the liquid, two-dimensionally permeating inhomogeneous nanoporous medium with altering porosity and pore size. This model allows us to analyze the correlation between the inhomogeneities of the media and the shape and transition of the front. The evolutions of the liquid front profile for nanoporous media with various parameters have been obtained using the program written in C++.

1. Introduction

In recent years nanoporous materials have become a subject of various scientific researches. Considerable attention is given to their application in biology and medicine. For example, nanoporous materials can be used for drug delivery [1, 2], immunoisolation [3], tissue engineering [4], as biological sensors [5], etc.

One of the topical problems in the theoretical studying of the nanoporous media are the transport processes [6]. It should be noted that transport processes in nanoporous systems are considerably more complex, than in homogeneous phases or even in macroporous systems [7]. The purpose of our work is to numerically model the motion of the front of the liquid, two-dimensionally permeating inhomogeneous nanoporous medium with altering porosity and pore size. Such model allows us to analyze how the inhomogeneity of a medium influences the shape and the transition of the liquid front.

2. Description of the numerical model

The capillary forces in the liquid front create the pressure $P_H = -\frac{2\sigma}{R}$, where σ is the surface tension coefficient of the liquid, R is the pore radius. The flowing through the medium creates the pressure in the liquid.

The presented model is based on the continuity equation for the incompressible flow $\nabla \vec{v} = 0$ and the approximation of Darcy's law $\vec{v} = -\gamma \nabla P$, where \vec{v} is the velocity of the flow and P is the pressure in the fluid. Their combination results in the linear differential equation (LDE):

$$\nabla(\gamma \nabla P) = 0 \quad (1)$$

with boundary conditions:



$$\begin{aligned}
P_0|_{y=0} &= 0 \\
P_H|_{y=H} &= -\frac{2\sigma}{R} \\
\frac{\partial p}{\partial n}|_{x=0} &= \frac{\partial p}{\partial n}|_{x=L} = 0
\end{aligned} \tag{2}$$

Here the coefficient γ describes the permeability of the porous medium [8]:

$$\gamma = \frac{\Omega R^2}{8\mu} \tag{3}$$

where Ω is the porosity of medium, R is the average pore radius and μ is the dynamic viscosity coefficient of the fluid.

The γ coefficient describes the structural properties of the nanoporous medium. By introducing the set of γ values as a matrix of the same size as the numerical scheme grid we are able to specify the γ value in every grid node. This allows us to take into consideration the inhomogeneity of the medium.

The numerical calculation procedure includes two steps:

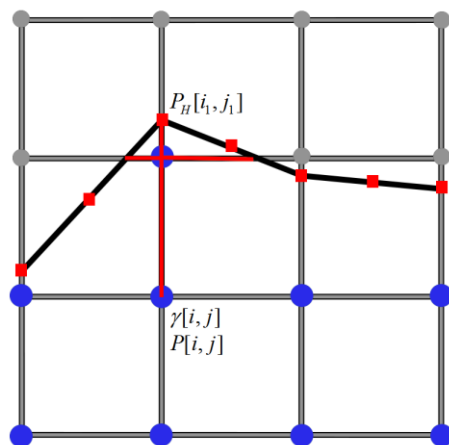


Figure 1. The numerical calculation procedure, step 1: solving LDE (1) by finite-difference method.

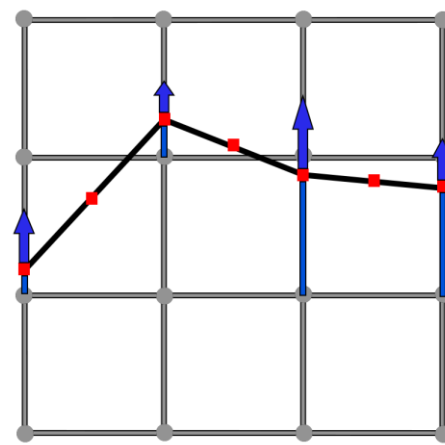


Figure 2. The numerical calculation procedure, step 2: translocation of the front and interpolation.

Firstly, by solving LDE (1) we obtain the pressure distribution in the medium's part which has been permeated by liquid. Secondly, on the basis of the derivative of the pressure we translocate the front points, which lie on the grid, and interpolate the results. Since a medium is inhomogeneous, the capillary pressure P_H changes with fronts motion and must be recalculated after each iteration using a matrix, which comprises the values of possible capillary pressures and also is of the same size as the grid.

3. Results

The computer simulation program, which numerically models two-dimensional motion of the front of the liquid, permeating inhomogeneous nanoporous medium, has been written in C++. The evolutions of the liquid front profiles for different inhomogeneous nanoporous media are demonstrated in the figures 3, 4, 5 and 6.

The following parameters were used for time evaluation: average pore size $\bar{R} = 10$ nm and parameters of the water $\sigma = 0.07$ N/m, $\mu = 0.8$ mPa s. In most cases porosity has been taken as constant $\Omega = 0.8$.

Darker areas in the figures' 3, 4, 5 and 6 backgrounds indicate smaller pore size and lighter, accordingly, larger.

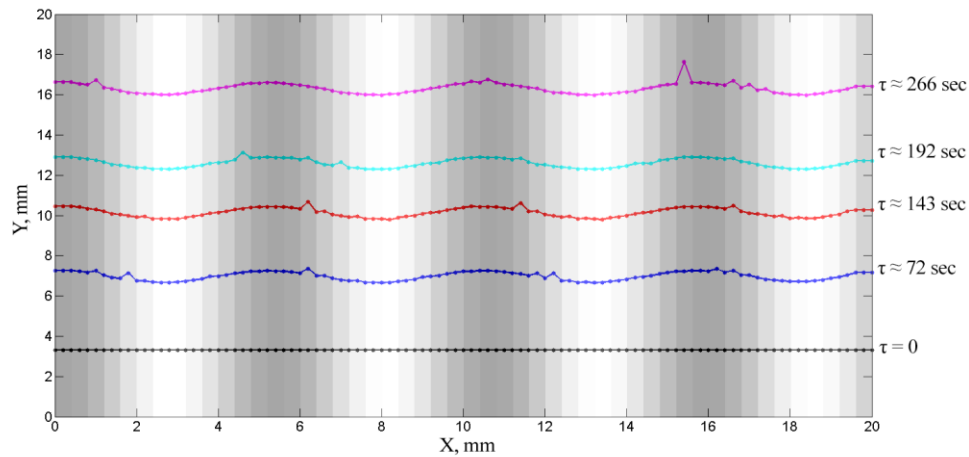


Figure 3. The evolution of the water front profile in case of pore size changing periodically in one direction: $R = \bar{R} + 3.5 \sin^2(kx)$ nm. The porosity of the medium is constant: $\Omega = 0.8$. Darker areas in the background correspond to smaller pore size and lighter ones, respectively, to larger.

Figure 3 shows the modification of the fronts shape in accordance with the alteration of the pore size in the medium, assuming that the porosity is constant. The evolution of the fronts shape in the medium in which both pore size and porosity vary can be seen at the figure 4:

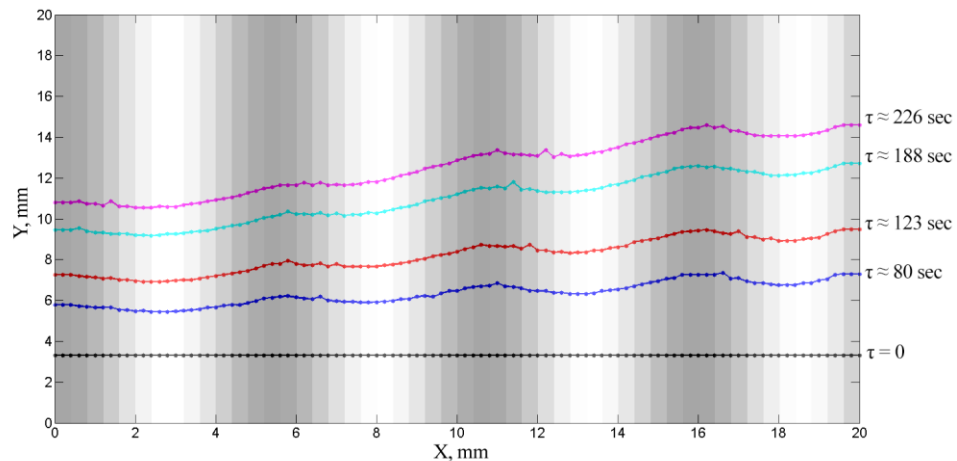


Figure 4. The evolution of the water front profile in case of pore size changing periodically in one direction: $R = \bar{R} + 3.5 \sin^2(kx)$ nm. The porosity of the medium Ω changes stepwise from 0.4 to 0.8 from left to right. Darker areas on the background correspond to smaller pore size and lighter ones, respectively, to larger.

If medium's porosity changes stepwise, the main characteristic of the modification of the fronts shape remains the same. However, the front moves faster in the parts of the medium with larger porosity, which leads to additional linear deviation of the front from its original shape. Also, in the areas with larger porosity the impact of the pore size variation is more considerable, which results in

more notable bending of the front in the mediums parts with larger porosity, if the pore size alters in the same way.

Figure 5 shows the evolution of the liquid front profile in the medium in which pore size vary in both directions:

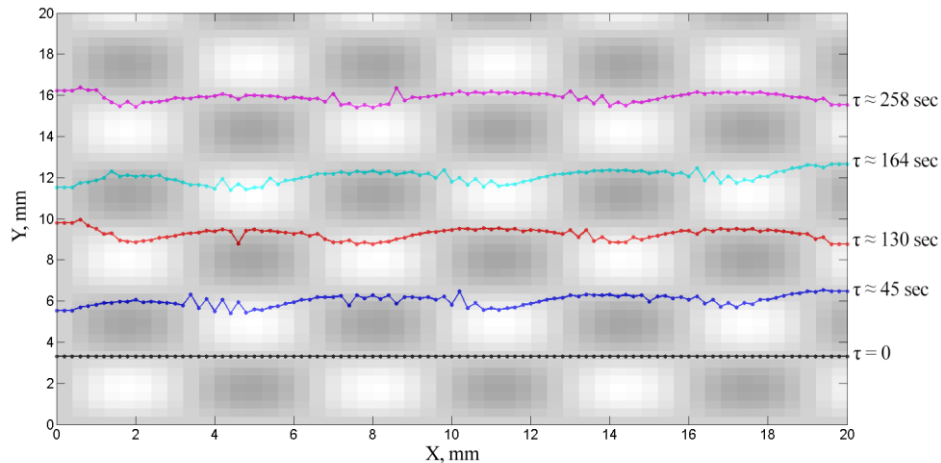


Figure 5. The evolution of the water front profile in case of pore size changing periodically in two directions: $R = \bar{R} + 3.5 \sin(kx) \sin(ky)$ nm. The porosity of the medium is constant: $\Omega = 0.8$. Darker areas in the background correspond to smaller pore size and lighter ones, respectively, to larger.

Both figure 3 and figure 5 show that if mediums porosity is constant, liquid flows faster through the areas with smaller pores, which results in bending of the front in accordance with the difference between the sizes of the nearby pores.

Figure 6 shows the evolution of the water front profile in the medium with random distribution of the pore size. As expected, fronts shape remains generally linear, with comparatively small deviations:

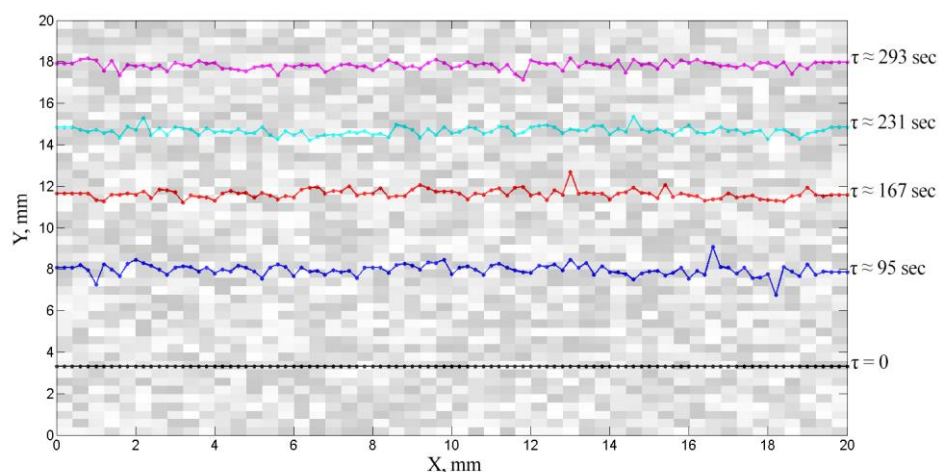


Figure 6. The evolution of the water front profile in case of pore size changing randomly from 10 to 13.5 nm. The porosity of the medium is constant: $\Omega = 0.8$. Darker areas in the background correspond to smaller pore size and lighter ones, respectively, to larger.

4. Conclusion.

The numerical model, which simulates the motion of front of the liquid, two-dimensionally permeating an inhomogeneous nanoporous medium, has been proposed. The evolutions of the water front profiles for different inhomogeneities of the media (such as pore size changing periodically in one or two directions and randomly) have been obtained and the time of water propagation has been evaluated.

In case of equally altering pore size the bending of the front is more notable in the parts of the medium with larger porosity. The stepwise changing of porosity also adds the additional linear deviation of the front from its original shape. If the porosity is constant, the front bends in accordance with the relation between pore sizes.

Acknowledgments

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