Drainage and impregnation capillary pressure curves calculated by the X-ray CT model of Berea sandstone using Lattice Boltzmann's method

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Abstract. The study deals with the features of the technique for simulating the capillary pressure curves of porous media on their X-ray microtomographic images. The results of a computational experiment on the immiscible displacement of an incompressible fluid by another in the pore space represented by a digital image of the Berea sandstone are presented. For the mathematical description of two-phase fluid flow we use Lattice Boltzmann Equation (LBM), and phenomena at the fluids interface are described by the color-gradient model.

Compared with laboratory studies, the evaluation of capillary pressure based on the results of a computational filtration experiment is a non-destructive method and has a number of advantages: the absence of labor for preparation of fluids and core; the possibility of modeling on the scale of very small core fragments (several mm), which is difficult to realize under experimental conditions; three-dimensional visualization of the dynamics of filling the pore space with a displacing fluid during drainage and impregnation; the possibility of carrying out multivariate calculations for specified parameters of multiphase flow (density and viscosity of fluids, surface tension, wetting contact angle).

A satisfactory agreement of the capillary pressure curves during drainage with experimental results was obtained. It is revealed that with the increase in the volume of the digital image, the relative deviation of the calculated and laboratory data decreases and for cubic digital cores larger than 1 mm it does not exceed 5%. The behavior of the non-wetting fluid flow during drainage is illustrated. It is shown that flow regimes under which computational and laboratory experiments are performed the distribution of the injected phase in directions different from the gradient of the hydrodynamic drop, including the opposite ones, is characteristic.

Experimentally confirmed regularities are obtained when carrying out calculations for drainage and imbibition at different values of interfacial tension. There is a close coincidence in the average diameters of permeable channels, estimated by capillary curves for different interfacial tension and pore network model. The differences do not exceed 15%.

1. Introduction

Capillary force plays a significant role at multiphase flows in a porous medium and an important characteristic in the study of hydrodynamic processes. The value of the capillary pressure is a function of the medium saturation by different phases and, in the first approximation, depends on the geometry of the pore space, the interfacial tension and the contact angle of wetting [1]. In laboratory conditions the most common methods for measuring capillary pressure curves are the mercury porosimetry [1], capillarimetry (or semipermeable membrane method) [2] and centrifugation [3]. The general drawbacks of these methods include such laborious stages as the preparation of fluids and the surface of pore channels, the long time of experiments on low permeable samples.

As an alternative to laboratory filtration experiments, the methods of numerical calculations on a digital microtomographic core images are being intensively developed in recent years. For computing resources optimization pore-network models (PNM) [4], in which the original digital image of pore space is associated with a model of spherical pores and cylindrical capillaries connecting them, are used. According to this model, with a given geometry of the pores and tubes capillary pressure is estimated by the Laplace formula. The increasing availability of high-speed computing technology and the compilers...
improvement make it possible to use a computational experiment on immiscible displacement of one incompressible fluid by another in pore-space, which is represented by the original digital image. The features of this method are described in detail in Sections 3.

The correspondence problem between the filtration parameters, which are calculated during computer modeling on the digital cores models of the order of 1 mm in size, and the values obtained in laboratory experiments on standard samples with a size of several centimeters is the subject of discussion in works of many authors [4, 5]. According to one of the most common approaches [4], the question of rescaling from the micro to the laboratory level is solved by finding a representative elementary volume of the digital image, in which the characteristics of the micromorphographic model reproduce the properties of the sample at a centimeter level. However, as shown in [5], this is not a universal approach in cases of a complex pore space structure, especially for carbonate reservoirs. Thus, using of simulation results on the digital cores for describing the properties of the specific reservoirs requires a particular methodological study, some theses of which are described in Ref [5].

The purpose of this paper is to verify the proposed approach, which consists in quantitative and qualitative data comparison with known experimental results and regularities, as well as testing the appropriateness and adequacy of this technique for typically small core fragments used in micromorphography, on the order a few millimeters. The sample of the study is a digital model of a natural sandstone with volume ~ 1 mm$^3$ which is representative in the laboratory scale for the coefficients of porosity and absolute permeability. This circumstance allows us to make a correct comparison of the calculated and experimental capillary pressure curves.

Compared with laboratory studies, capillary pressure estimation, which is based on the results of a computational filtration experiment, is a non-destructive method and has a number of advantages: the labor costs absence for preparation of fluids and core; the possibility of modeling on the scale of very small core fragments (several mm), which is difficult to realize under laboratory conditions; three-dimensional visualization the pore space filling with a displacing fluid during drainage and imbibition; the possibility of carrying out multivariate calculations for various parameters of multiphase flow (density and viscosity of fluids, surface tension, contact angle).

2. The sample of study.

The sample of the study is the Berea sandstone. This type of sandstone is standard for laboratory testing of oil and gas industry processes and has been used in various works, among which Tsuji T. et al. [6] Blunt M. et al. [7], Berg S. et al. [8]. According to the mineralogical studies given in [8], Berea sandstones consist of quartz, feldspar, calcite and clay minerals.

A digital model of pore-space from the Imperial Colledge London open library [http://www.imperial.ac.uk/earth-science/research/research-groups/perm/research/pore-scale-modelling/micro-ct-images-and-networks/berea-sandstone/] is represented by a cubic binarized three-dimensional micromorphographic image with size of 400 voxels and a resolution of 3.2 μm. Images of Berea sandstone in 3D and 2D projections are shown in figure 1. The porosity coefficient of this fragment is 19.6%. The absolute permeability tensor is practically isotropic, since the fraction of its isotropic component $K_{iso} = 0.670 \text{ μm}^2$ [9, 10] is more than 92%. The cube fragment of Berea sandstone with a size of 1 mm is representative, and this, in fact, is slightly smaller than the volume of the image we use, whereas experiments for the capillary pressure curves measuring were carried out on a 160 mm$^3$ sample (10 mm × 4 mm × 4 mm).
3. Materials and methods.

3.1. Method for capillary pressure curves measuring during drainage and imbibition.

In this paper for the capillary pressure curves determination we carry out a computational experiment on the immiscible displacement of one incompressible fluid by another. At the initial time, the pore space is completely filled with the wetting phase. The computational experiment consists of several stages. The first consists in injecting a nonwetting phase into the sample and, consequently, displacing the wetting fluid from it (drainage). The injected nonwetting fluid is fed to the leftmost side (input boundary), which is perpendicular to the OX axis, and the selection of two liquids occurs through the rightmost section (the exit boundary), also perpendicular to the OX axis. The other four outer faces of the computational domain are impermeable to fluids. We carry out the experiment at various pressure differences between the inlet and outlet sections. The minimum pressure drop at which the displacement process begins is a threshold. At the finishing of each mode, i.e. when a flow rate of the wetting phase through the outlet boundary is zero, we make a stepwise increasing in pressure at the inlet section, and the drainage process continues. The drainage process finishes when the wetting phase displacement with a further increase in pressure terminates.

At the next stage, the pressure at the input boundary is reduced. All cells in the outlet section that are related to the pores being filled with the wetting phase. During this experiment, the wetting phase displaces the nonwetting through the inlet region of the sample, i.e. we simulate the imbibition process. When the flow rate of the nonwetting phase through the inlet section is zero, the pressure on it decreases in a stepwise manner, after which the imbibition continues. In the latter stage of imbibition, the pressure difference between the input and output boundaries are equal. After the calculations under the given conditions, the experiment is completed.

The measurement of sample saturation by wetting phase at each drainage and imbibition regime is carried out under the condition when wetting and nonwetting phases are not displaced, respectively, and the resulting pressure drop is therefore capillary.

3.2. Lattice Boltzmann method.

The paper considers a two-phase isothermal flow of immiscible incompressible liquids in porous medium. The Lattice Boltzmann method or Lattice Boltzmann Method equations (abbreviated LBE) are used to describe the flow of liquids. This mathematical model is described in many works [11, 12], so we will not give a detailed mathematical description of it, but dwell only on the basic assumptions.

In the framework of LBE, the flow of a medium is considered as dynamics of a particles ensemble with a given finite number of possible velocities. The flow domain is represented by grid with a square or cubic cell shape. The set of these form a lattice. During a time step \( \Delta t \) particles without interaction with each other can make one act of transition between adjacent lattice sites. One-particle distribution functions \( f(r, u, t) \) are used to describe the state of the system at each grid node. This function shows the part of particles at time \( t \) located in the vicinity of point \( r(x,y,z) \) with coordinates from \( x \) to \( x+\Delta x \), from \( y \) to \( y+\Delta y \), from \( z \) to \( z+\Delta z \) and with velocity range from \( u(x, u_y, u_z) \) to \( u(x, u_y+\Delta u_y, u_z, u_z) \).
For a two-dimensional flow domain, for example, a discrete set of velocities D2Q9 is given as follows: $e_1 = c(0,0); e_2 = c(1,0); e_3 = c(0,1); e_4 = c(-1,0); e_5 = c(0,-1); e_6 = c(1,1); e_7 = c(-1,1); e_8 = c(-1,-1); e_9 = c(1,-1)$, where $c = \frac{\Delta t}{\Delta l}$ – the lattice speed, $\Delta l$ – the grid spacing. Each velocity vector from a given set $e_i$ (i = 1..9) corresponds to the distribution function $f_i(r,t)$, depending only on $t$ and $r$. In a case of 3D we use D3Q19 model.

The dynamics of the particles ensemble of each fluid is described in several stages. The first is called streaming step. At this stage, the particles move to neighboring nodes during time $\Delta t$, and the direction of the motion speed does not change. The second stage deals with the collision process of particles, as a result of which the distribution function tends to the equilibrium state. The third stage describes the interface interaction between two fluids and between fluids and the solid phase. The distribution function evolution for each fluid in time and space is described by equation (1):

$$f_i^k(r + e_i \Delta t, t + \Delta t) = f_i^k(r, t) + \left( (\mathbf{Q}^k_i \cdot \mathbf{r}) + (\mathbf{Q}^k_i \cdot \mathbf{r}) \right),$$

where $k = o, w$ – are oil and water.

$(\mathbf{Q}^k_i)$ is a collision operator. There are two main models, which describe collision of particles – Single Relaxation Time (SRT) [11-13] and Multi Relaxation Time (MRT) [13]. The results obtained with MRT model use have a more exact match when comparing with known analytical solutions [13] (for example, Couette flow) than SRT model. So, that is why in our work we use MRT approach.

The relaxation coefficient $\tau$ is the determining parameter in the SRT and MRT models and controls kinematic viscosity according to the equation (2):

$$\mu^k = \left( \frac{2 \tau^k - 1}{6} \right) \frac{\Delta l^2}{\Delta t}$$

In contrast to the classical equations of the fluid and gas mechanics (for example, the Navier-Stokes equations), where the solution is sought in the "pressure-velocity" variables, the LBE are solved in the "density-velocity" variables. The macroscopic density and velocity in the cell of domain are calculated using (3) and (4) formulas, respectively:

$$\rho^k(r, t) = \sum_{i=1}^{9} e_i f_i^k(r, t)$$

$$u^k(r, t) = \frac{1}{\rho^k} \sum_{i=1}^{9} e_i f_i^k(r, t)$$

The pressure $p$ in LBE, which is produced by each fluid, is related to its density by the following relation: $p^k = \frac{\rho^k c^2}{3}$ [11, 12].

The phenomena at the interface of fluids are described using the color-gradient method [14]. It consists of several types:

1) calculation of the color field gradient $\mathbf{g}$, which components are calculated by the formula:

$$g(r, t) = \sum_{i=1}^{9} e_i (f_i^o (r + e_i \Delta t, t) - f_i^w (r + e_i \Delta t, t))$$

Traditionally, one fluid is red, and the second is blue;

2) description of the surface tension effects on the interface between fluids:

$$(\mathbf{Q}^k) = \frac{A}{\rho} |\mathbf{g}| (2 \cdot \cos^2 (\alpha_1) - 1),$$

where parameter $A$ controls surface tension $\sigma$, $\alpha_1$ is an angle between $\mathbf{g}$ and $e_i$ direction.

3) «recoloring» step – modification of $f_i^k$ after solving equation (1):

$$f_i^o = \frac{\rho^o}{\rho} f_i + \beta \frac{\rho^o}{\rho} \cdot f_i^{eq} \cdot \cos (\alpha_1)$$

$$f_i^w = \frac{\rho^w}{\rho} f_i - \beta \frac{\rho^w}{\rho} \cdot f_i^{eq} \cdot \cos (\alpha_1)$$
where $\rho = \rho^o + \rho^w$, $f_i = f_i^o + f_i^w$, $f_i^w$ is an equilibrium function distribution [11], calculated at a density $\rho$ and zero velocity. The parameter $\beta$ influences on thickness of the fluid interface. In this paper, its value is 0.8 and can not exceed 1.

On the internal solid and external impermeable boundaries of the flow domain we use "bounce back" conditions [11, 12]. At the input and output boundaries, the fluid pressure is known and the velocity components normal to the boundary is equal to zero. In LBE, such conditions are given by Zow and He equations [15].

The densities of the wetting and nonwetting phases in all computational experiments are 1000 kg / m$^3$, and the viscosity is 2 mPa·s and 1 mPa·s, respectively. Accoding to [8], the contact wetting angle is 0°. This model assumes a constant temperature, chemical composition, no deformation of the skeleton and the density of liquids in the used pressure range.

4. Results and discussion

To verify the method proposed in Sections 2 and 3, we perform a comparison of the capillary drainage pressure curves, the calculation of which was carried out on the digital core samples with dimensions of 100, 200, 250 and 300 voxels, with the laboratory experiment results (figure 2). The digital core tested in our study was equal to a sample for which laboratory measurements of porosity, absolute permeability, and the capillary pressure curves by mercury porosimetry were made in Ref. [8]. The surface tension in the calculations and experiment was 28.8 mN / m. For each curve, the average of the relative deviation absolute value was calculated using the following formula: 

$$\Delta^i = \frac{100}{N} \sum_{i=1}^{N} \left| \frac{S^i_{\text{model}} - S^i_{\text{experiment}}}{S^i_{\text{model}}} \right|,$$

where $N$ is the number of pressure measurements (in our case $N = 11$); $S^i_{\text{model}}$ and $S^i_{\text{experiment}}$ – the wetting phase saturation at $i$-th capillary pressure, measured in the computational and laboratory experiments, respectively; $\alpha$ indicates the size of the digital core. According to the results shown in figure 2, $\Delta^{100} = 10.2 \%$, $\Delta^{200} = 8.5 \%$, $\Delta^{250} = 5.0 \%$, $\Delta^{300} = 3.3 \%$. The fact that $\Delta$ for model with size of 250 voxels and above does not exceed 5%, the cubic digital cores of this sample, taken with a resolution of 3.2 μm and sizes of more than 1 mm, can be considered representative on a laboratory scale for measuring the capillary pressure of Berea sandstones. Note that the size of the representative volume is a specific value for each type of pore-space and can even exceed the dimensions of the digital model.

Figure 2. Comparison of the capillary pressure curves measured experimentally and calculated on the digital cores cubic fragments with sizes of 100, 200, 250 and 300 voxels
Figure 3 illustrates the dynamics of pore space filling with a non-wetting phase during drainage for the 100-voxel fragment. In figure 3b, 3c and 3d, the yellow arrow indicates areas in which the flow directions of the non-wetting phase differ from the created pressure gradient (i.e. upward) including the opposite ones (figure 3c and figure 3d). Analyzing the flow pattern in figure 3a and figure 3b, it can be noted that the interface coordinate, which is closest to the exit cross section, has not changed, and the displacement of the wetting phase occurs approximately perpendicular to the hydrodynamic pressure gradient. Such effects are a distinguishing feature of the regimes in which "capillary" fingers are formed and arise in cases when capillary number is less, than $-3$ [6].

Figure 3. Visualization of non-wetting phase flow during drainage. $S_{nw}$ - the volume fraction of the non-wetting phase in the pore space: a – 0.13; b – 0.17; c – 0.25; d – 0.48

Further, we investigate the trend of increasing capillary pressure in the series of computational experiments with different values of the interfacial tension $\sigma = 7.7$ mN/m, 14.4 mN/m, 28.8 mN/m. The calculations of drainage and imbibition curves were performed on a digital core of a cubic shape with sizes of 250 voxels. The results (figure 4 and Table 1) show that the drainage and imbibition curves measured at the same interfacial tension are not equivalent to each other, i.e., the hysteresis is manifested. Reduction of interfacial tension causes a decrease in capillary pressure, resulting in both the drainage and the imbibition curves are shifted to smaller values. The values of the residual saturation of a wetting phase (column 3 in Table 1) and the threshold drainage capillary pressure (column 2 in Table 1) are reduced by decreasing the interfacial tension, and the residual saturation with a nonwetting phase (column 4 in Table 1) increases with impregnation. Figure 5 shows the distribution of the residual nonwetting phase in the sample when impregnated for 14.4 mN/m. As can be seen from figure 5, the liquid is mostly presented the closed globules enclosed in the pore channels, some of them are shown in a larger size on the right-hand side of the figure 5. However, the results obtained by the above-mentioned method, are in agreement with experimental results [16].
We made comparison of the pore channels average diameters, estimated on the drainage results using the Laplace formula \( P_c = \frac{2\sigma}{R} \) and in direct measurement by PNM [6]. The results are demonstrated in columns 5 and 6 of Table 1 (the relative deviation from the average pore diameter by PNM is indicated in parentheses in column 5). Since the drainage curve at the interfacial tension \( 28.8 \text{ mN/m} \) was successfully compared with the experimental \( (\Delta = 5.0\%) \), and the calculated diameters for different interfacial tensions are close (column 5), we can conclude that Laplace's formula estimates the pore size distribution with sufficient accuracy.

**Table 1.** Characteristics of capillary pressure curves at different interfacial tensions

| Interfacial tension, mN/m | Threshold pressure, Pa | Residual saturation of a wetting phase, relative units | Residual saturation of a nonwetting phase, relative units | Average pore diameter in LBM (the relative deviation from PNM), \( \mu m \) | Average pore diameter in PNM [6], \( \mu m \) |
|---------------------------|------------------------|------------------------------------------------------|------------------------------------------------------|-------------------------------------------------|-----------------|
| 28.8                      | 1300                   | 0.265                                                | 0.143                                                | 18.1 (–9.5 %)                                   |                 |
| 14.4                      | 500                    | 0.245                                                | 0.16                                                 | 17.4 (–13 %)                                    |                 |
| 7.7                       | 350                    | 0.215                                                | 0.18                                                 | 18.1 (–9.5 %)                                   | 20              |

**Figure 4.** Capillary drainage and impregnation pressure curves at various interfacial tension
5. Conclusions
In the work, testing and approbation of the capillary pressure curves measuring technique by microtomographic digital images was carried out. We obtained a satisfactory agreement with the experimental data. It was revealed that with the digital image volume increasing, the discrepancy between the calculated and experimental data decreases. The pore channels system of Berea sandstone in a cubic digital model larger than 1 mm is representative in laboratory scales for the estimation of capillary pressure values. The pictures of the non-wetting liquid flow during drainage are illustrated. It was shown that for the flow regimes under which the computational and laboratory experiments are carried out, the directions of nonwetting phase flow differ from the gradient of the hydrodynamic pressure drop, including the opposite ones. During drainage and imbibition calculations at different values of interfacial tension, we obtained regularities, which are confirmed experimentally. Comparison of average pore diameters estimated by capillary curves for different interfacial tension and pore-network model is satisfactory, the discrepancy does not exceed 15%.

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Figure 5. Distribution of residual non-wetting phase at 14.4 mN / m. Some of isolated globules are shown on the right-hand side in larger scale
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