Pore-Scale Modeling Of Two-Phase Flows At Various Surface Tensions And Wetting Contact Angles

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Abstract

The paper studies the features of two-phase flows in a porous medium at different values of surface tension and contact angles of wetting. As an example, an artificially created digital two-dimensional model of a porous medium with a random distribution of impermeable obstacles of rhomboid, quadratic and rectangular shape is considered. In order to model the multiphase flow, the Boltzmann lattice equations and the color field gradient model are used.

Computational experiments are carried out to displace the wetting phase saturating the porous space at the initial instant of time by injecting a nonwetting liquid at various interfacial tensions and the wetting properties of a skeleton. Based on the calculations, it was found that at very low values of the capillary pressure in the porous medium, the "fingers" and isolated globules of the injected non-wetting phase are formed in comparison with the hydrodynamic drop. At comparable values of capillary and hydrodynamic pressures, the uncharged liquid uniformly fills the pore space, but a significant part of the wetting phase remains stationary. It was shown that the result of the capillary resistance decrease is the flow rate increase of the wetting liquid through an outlet section. The intensification of the flow is mainly manifested after the breakthrough of injected liquid from the sample and it is increased at capillary pressure decrease.

Key words: mathematical modeling, porous media, capillary pressure, wetting contact angle, surface tension
1. INTRODUCTION

Capillary phenomena have a significant effect on two-phase flows in porous media and, in the first approximation, they depend on the radius of their pore channels, the surface tension at the interface of liquids and wetting properties. In oil and gas industry, the most pronounced effects from the modification of the capillary resistance forces are manifested in the change of mobile fluid volume saturating a porous medium at the initial instant of time and the rate of liquid extraction [Abramzon A.A., Zaichenko L.P., Feingold S.N. 1988;Derkach S.R., Berestova G.I., Motyleva T.A. 2010;Xu X., Jeong T. O., Xiao F., et al. 2014;Gimatudinov Sh. K. 1983;Zakirov T. R., Galeev A. A., Konovalov A. A., Statsenko E. O. 2015].

In this paper, a quantitative assessment of changes concerning flow processes in a porous medium as the result of capillary pressure change is carried out at the scale of the pore channels. Within this approach, the cell of the computed area is either filled with a fluid, or is a skeleton (the grid step makes several μm) [Zakirov T. R., Galeev A. A., Korolev E. A. et al. 2016;Chen S., Doolen G. 1998]. With this approach, in addition to volumetric flow parameter calculation, it is possible to observe the movement of the interface between two fluids directly in the pores, in contrast to the saturation jump at the modeling in reservoir scale. The need for a detailed study of fluid distribution structure in the pore space in time is conditioned by the dependence of displacement indices on the specificity of the interphase front motion, which, in its turn, depends directly on the pore geometry. The purpose of this work is to identify the features of a two-phase flow in the pore scale at different values of interfacial tension and the contact angle of wetting.

2. METHODS

2.1. Mathematical statement of the problem

The paper deals with a two-phase isothermal flow of non-mixed incompressible liquids. In order to describe the flow of fluids, they use Lattice Boltzmann Method (LBM) is used. This mathematical model is described in many works [Succi S. 2001;Pan C., Luo L. S., Miller C. T. 2006;Aslan E., Taymaz I., Benim A. C. 2014;Niu X., Munekata T., Hyodoa Sh. et al. 2007;Reis T., Phillips T. N. 2007;], therefore we will not give a detailed mathematical description of it, but we will dwell only on the basic statements.
In the framework of LBM, the flow of a medium is considered from the point of view of particle ensemble dynamics with a given finite number of possible velocities. The flow area is divided by a grid with cells, usually of a square or a cubic shape. The collection of these cells is a lattice. During a step in time $\Delta t$ particles can perform one act of transition between adjacent lattice sites without the interaction with each other. As variables describing the state of a system at each site of the grid, one-particle distribution function $f(r, u, t)$ are used. This function shows the fraction of particles at time $t$ located near the point $r$ $(x, y, z)$ with the coordinates from $x$ to $x + \Delta x$, from $y$ to $y + \Delta y$, from $z$ to $z + \Delta z$ and with the velocities in the range from $u$ $(u_x, u_y, u_z)$ to $u$ $(u_x + \Delta u_x, u_y + \Delta u_y, u_z + \Delta u_z)$.

For a two-dimensional flow region, a discrete set of velocities $D2Q9$ is used, which is defined as follows: $e_1 = c \cdot (0,0)$; $e_2 = c \cdot (1,0)$; $e_3 = c \cdot (0,1)$; $e_4 = c \cdot (-1,0)$; $e_5 = c \cdot (0, -1)$; $e_6 = c \cdot (1,1)$; $e_7 = c \cdot (-1,1)$; $e_8 = c \cdot (-1, -1)$; $e_9 = c \cdot (1, -1)$, where $c = \frac{\Delta l}{\Delta t}$ – the base velocity ($\Delta l$ – grid step).

Each velocity vector from the given set $e_i$ $(i = 1..9)$ is corresponded with the distribution function $f_i(r,t)$, depending only on $t$ and $r$.

The description particle ensemble dynamics of each of the fluids is performed in several stages. The first stage is the "streaming step". At this stage, the particles move to neighboring nodes during time $\Delta t$, and the direction of the speed of motion does not change. At the second stage, the process of collision of particles ("collision step") is considered, after which the particle distribution function tends to an equilibrium state. The third stage describes the interaction of fluids with each other at the interface, as well as with the solid phase. The evolution of the distribution function of each fluid in time and space is described using the equation (1):

$$f_i^k (r + e_i \Delta t, t + \Delta t) = f_i^k (r, t) + (\Omega_i^k (r, t))^1 + (\Omega_i^k (r, t))^2 \tag{1}$$

где $k = 1, 2$ where $k = 1, 2$ indicates the type of fluid, i.e. the wetting and non-wetting phases, respectively.

Depending on the form of a collision operator presentation $(\Omega_i^k)^1$, one distinguishes SRT-model (Single relaxation time) and MRT model (Multi relaxation time) [Huang J., Xiao F., Yin X. 2014; Zou Q, He X. 1997]. MRT model is used in this paper.
The relaxation parameter $\tau^k$ is the determining parameter in SRT and MRT model. It serves to control the kinematic viscosity $\mu^k$ of the fluid and is related to it by the relation (2):

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

(2)

The equations in LBM method are solved in the variables "density-velocity". The macroscopic density and velocity components of each fluid in the cells are calculated by the formula (3) and (4):

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

(3)

$$u^k (r, t) = \frac{1}{\rho^k} \sum_{i=1}^{9} \varepsilon_i f^k_i (r, t)$$

(4)

The pressure $p^k$ in LBM method, produced by each fluid is related to its density by the following relationship: $p^k = \frac{\rho^k c^2}{3}$ [8].

In order to describe the phenomena occurring at the fluid interface, this paper uses Color-field method [13, 14]. It consists of several stages:

1) The calculation of the color field gradient $g$, the components of which are calculated by the following formula:

$$g(r, t) = \sum_{i=1}^{9} \varepsilon_i (f^2_i (r + \varepsilon_i \Delta t, t) - f^1_i (r + \varepsilon_i \Delta t, t)).$$

(5)

Traditionally, one of the fluids is assigned a red color, and the other one is blue;

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

$$(\Omega^k_r)^2 = \frac{A}{2} |\mathbf{g}| (2 \cdot \cos^2(\alpha_i) - 1),$$

(6)

where $A$ is the parameter controlling the surface tension, $\alpha_i$ is the angle between the vector $g$ and the direction $e_i$. 
3) «Recoloring» step – the modification of the function \( f_i^e \) after the following equation

\[
(f_i^2)^* = \frac{\rho^o}{\rho} f_i + \beta \frac{\rho^o \cdot \rho^w}{\rho} f_i^{eq} \cdot \cos(\alpha_i),
\]

\[
(f_i^1)^* = \frac{\rho^w}{\rho} f_i - \beta \frac{\rho^o \cdot \rho^w}{\rho} f_i^{eq} \cdot \cos(\alpha_i)
\]

is the equilibrium distribution function [10,11], calculated for the density \( \rho \) and the velocity equal to zero. The parameter \( \beta \) controls the thickness of the fluid interface. In this paper, its value makes 0.8 (and can not exceed unity).

As the boundary conditions on the solid and outer impermeable boundaries of the flow region, they use "bounce back" conditions [8,9], which are the analogues of the conditions for non-flow and the adherence of a liquid in the classical statement of the problem. At the input and output boundaries, the fluid pressure and the velocity components normal to the boundary, which make zero, are assumed to be known. In LBM, such conditions are given by the means of the relations \( 3_{oy} \) and \( Xe \) [15].

The mathematical model was developed and implemented in the form of a program code with the support of RFFI grant mole_a 16-35-00155.

2.2. Study sample

The calculated flow region of two liquids is an artificially created two-dimensional digital model of a porous medium with a random distribution of impermeable obstacles (a framework) of a rhomboid, quadratic and rectangular shape (Fig. 1). The grid size makes 800 cells along the horizontal axis OX and 300 cells along the vertical axis OY; the grid cells have a square shape with a side of 5 \( \mu \)m. The numerical values on the coordinate axes of Fig. 1 are given in \( \mu \)m.
3. RESULTS AND DISCUSSION

3.1. Calculation experiment parameters

We give the framework a hydrophobic property as input data, i.e. the fluid that saturates at the initial instant of time will be considered as wetting, and the injected liquid will be non-wetting. A series of computational experiments is performed to displace the wetting fluid by injecting non-wetting (draining) one for various values of surface tension and wetting contact angle, indicated in Table. 1. The left side of the flow region is the input one, the right side is the output one; The lower and the upper faces are impermeable. The injected liquid is fed to the left side of the sample at a constant pressure drop between input and output boundaries of 5 kPa. Fluids flow through the right side, the pressure on which is a constant one during the experiment. The calculations are stopped when the porous medium does not have a mobile wetting phase any longer.

The densities of the liquids are equal and amount to 1000 kg/m³; the viscosity of the wetting and non-wetting phases $\mu_1 = 10$ mPa s and $\mu_2 = 1$ mPa s, respectively.

<table>
<thead>
<tr>
<th>Experiment №</th>
<th>Surface tension $\sigma$, mN / m</th>
<th>Limiting wetting angle $\theta$, grades</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>35.00</td>
<td>10</td>
</tr>
<tr>
<td>2</td>
<td>23.00</td>
<td>20</td>
</tr>
<tr>
<td>3</td>
<td>12.00</td>
<td>30</td>
</tr>
<tr>
<td>4</td>
<td>4.00</td>
<td>45</td>
</tr>
<tr>
<td>5</td>
<td>1.50</td>
<td>60</td>
</tr>
</tbody>
</table>

The calibration of the mathematical model described in p. 1.1 was carried out at $\tau^1 = 1$ and $\tau^2 = 0.55$. The parameter $A$ in formula (6), controlling the surface tension, was chosen for each variant of the calculation on the basis of the problem solution about the
pressure drop from different sides of the spherical drop ("Bubble test") using Laplace's formula [13].

The wetting effects at the liquid / liquid / solid phase interface are described by assigning a specific density value $\rho_s$ to the "solid" cell. Figure 2 shows cases in which the density of the framework is 500 kg/m$^3$ (Fig. 2a), 0 kg/m$^3$ (Fig. 2b) and 500 kg/m$^3$ (Fig. 2c) with the density of each fluid of 1000 kg/m$^3$.

![Fig. 2. Wetting contact angles at different $\rho_s$:](image)

- $a$ - 500 kg / m$^3$; $b$ - 0 kg / m$^3$; $b$ - 500 kg / m$^3$

The calculations were carried out at HP Z640 computer station with the support of the program for competitiveness increase of the Kazan Federal University among the world's leading research and educational centers.

3.2. Numerical results

For each variant of calculation, an approximate estimate of the capillary pressure in the sample was made with the radius of the pore channel cross section $R = 20 \mu m$ according to the formula: $P_C = \frac{2\sigma \cos(\theta)}{R}$. The rounded values of this value from the first to the fifth experiment make 3.5 kPa, 2.2 kPa, 1 kPa, 0.3 kPa and 0.075 kPa, respectively.

The features of two-phase flow are considered before and after the breakthrough of the injected phase through an outlet section of the sample. Fig. 3 and Fig. 4 show the picture of pore space filling by the non-wetting phase for the computational experiments No. 1 and No. 5, respectively, when the front of coordinate displacement $x_f$ along the horizontal axis is equal to 1000 $\mu m$ (200 cells), 2000 $\mu m$ (400 cells), 3000 $\mu m$ (600 cells), 4000 $\mu m$ (800 cells) also at the end of the calculations (the displacement front is the interface between two phases closest to the output cross section). According to the data obtained, the surface tension and the contact angle of wetting make a significant

![Figure 3 and Figure 4 showing pore space filling](image)
influence on the structure of fluid distribution in the pore space due to the heterogeneity of its structure. With the variant of calculation No. 1 (Fig. 3), the hydrodynamic forces resulting from the pressure drop between the inlet and the outlet sections of 5 kPa are comparable to the forces of capillary resistance. In this mode, the displacement phase does not only tend to the output section, but it also spreads in all directions. On Fig. 3, such sections are marked by circles. During the experiment No. 5 (Fig. 4), the capillary resistance with respect to the hydrodynamic pressure drop is insignificant. The flow occurs predominantly towards the exit section, "fingers" and isolated globules of the injected fluid are developed (marked on Fig. 4 by circles) because of a weak intermolecular bond. According to Fig. 3d and Fig. 4d, it can be noted that with the surface tension and the wetting forces decrease, the volume of the stationary displaced liquid also decreases. The stationary phase is localized in so-called capillary traps and is expressed in the calculation No. 1 particularly distinctly (Fig. 3d).
Fig. 3. The distribution of the injected phase in the pores at $\sigma = 35$ mN/m, $\theta = 10^\circ$:

- a - $x_I = 1000 \, \mu m$;
- b - $x_I = 2000 \, \mu m$;
- c - $x_I = 3000 \, \mu m$;
- g - $x_I = 4000 \, \mu m$;
- d - the end of the experiment;

black - framework; white - pumped phase, gray - displaced phase
Fig. 4. Distribution of the injected phase in pores at $\sigma = 1.5$ mN/m, $\theta = 60^\circ$:

- a - $x_f = 1000 \mu\text{m}$;
- b - $x_f = 2000 \mu\text{m}$;
- c - $x_f = 3000 \mu\text{m}$;
- g - $x_f = 4000 \mu\text{m}$;
- d - the end of the experiment;

black - framework; white - pumped phase, gray - displaced phase
The flow pattern of two liquids, shown on Fig. 3 and Fig. 4, can be described numerically in the form of graphs of saturation dependencies of the sample by the pumped phase from the displacement front coordinate (Fig. 5) for each calculation variant. According to the curves shown on Fig. 5, it can be concluded that during the capillary effects decrease, the efficiency of filling the pore space with a non-wetting liquid also decreases. At the moment of its break through an output section, the saturation of the sample from the first to the fifth makes 0.587, 0.577, 0.529, 0.498 and 0.483, respectively.

**Fig. 5.** The saturation of the sample by the pumped phase at different coordinates of displacement front

Let us consider the influence of capillary effects on the dynamics of the wetting phase displacement. Figure 6 shows the graphs of the displaced phase accumulated volume in time for each calculation variant. The vertical black lines on Fig. 6 show the moments of injected liquid breakthrough from the sample for each computational experiment. It is seen from Fig. 6 that with the framework surface tension and wettability reduction, the breakthrough occurs in fewer time steps, which for the first to fifth calculations make 131,000, 110,000, 100,000, 93,000 and 89,000, respectively.

The curves on Fig. 6, corresponding to the calculations from the second to the fifth one, do not differ significantly until the moment of breakthrough. With these modes of multiphase flow, the injected phase, first of all, fills the large channels, in which the capillary resistance is small, and only then the pores are of smaller diameter (the structure of the flow depends on the geometry of the pore space obviously). The displacement of the fluid that saturates the sample at the initial instant of time from the
fine pores occurs predominantly after reaching the pumped phase of the output section. Thus, the influence of the surface tension and the wetting contact angle on the intensification of the flow is manifested mainly after a breakthrough, and its intensity increases with capillary resistance decrease.

The curve obtained during the calculation of No. 1 stands out on Fig.6. As was already shown on Fig. 3d, the volume of the immobile liquid is significant for the experimental parameters corresponding to this regime and, according to the results of calculations, it makes 22%, while for the remaining variants of calculation this value is at the level of 7-8%.

![Fig. 6. Accumulation dynamics of the wetting phase in time at various calculation options](image)

4. CONCLUSIONS

The studies have been carried out to identify the changes of two-phase fluid flow behavior in a porous medium due to the change in the interfacial tension and the contact angle of wetting. It was shown that at very low values of capillary pressure in the porous medium, the "fingers" and isolated globules of the injected phase are formed in comparison with the hydrodynamic drop. At comparable capillary and hydrodynamic pressures, the non-wetting fluid fills the pore space more efficiently, but a significant portion of the wetting phase that initially saturates the sample remains immobile.
The result of the surface tension and the contact angle decrease, the increase of the displaced phase flow velocity through an outlet cross section is observed. The intensification of the flow is mainly manifested when a non-wetting liquid breaks from the sample and increases with capillary pressure decrease.

5. SUMMARY

The mathematical model and the procedure of the computational experiment carrying out presented in this paper can be adapted for digital micro tomographic models of porous media. The obtained results in this paper can be valuable during the use of surface active substances evaluation that reduce the surface tension in an oil-saturated reservoir during flooding in the oil and gas industry.

6. ACKNOWLEDGEMENTS

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