Examination of Clastic Oil and Gas Reservoir Rock Permeability Modeling by Molecular Dynamics Simulation using High-Performance Computing

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Abstract. "Digital rock" is a multi-purpose tool for solving a variety of tasks in the field of geological exploration and production of hydrocarbons at various stages, designed to improve the accuracy of geological study of subsurface resources, the efficiency of reproduction and usage of mineral resources, as well as applying of the results obtained in industry. This paper presents the results of numerical calculations and their comparison with the full-scale natural examination. Laboratory studies have been supplemented with petrographic descriptions to deepen an insight into behaviors of the studied rock material. There is a general tendency to overestimate the permeability, which may be associated with the application of a rather crude resistive model for assessing permeability and owing to the porous cement has not been considered.

Keywords: Digital Rock Model · High-Performance Computing · Clastic Oil and Gas Reservoir's Rock · Molecular Dynamics.

1 Introduction

Petroleum well cores examinations are among the most costly stages of development of oil and gas. Its partial replacement by the numerical experiments can provide significant economic benefits[1]. 3D-reconstruction of the rock microstructure problem arises within a framework of mathematical modeling of porous media macroscopic properties[2-4]. And the relation between the geometry of the microstructure and macroscopic physical properties, recently, arises interest in research teams. Permeability of porous materials is one of the macroscopic parameters of practical interest, and its measurement is important for predicting flows on macrolevel[5]. Significant advances in obtaining maps of interstitial space have been made recently. The usage of high-performance computing technology has accelerated the development and the use of tools "digital rock" in addition to the physical laboratory measurements.

The method of molecular dynamics is one of the promising approaches for building the mathematical model of the macroscopic properties of porous media and for the 3D-reconstruction of the rock microstructure. The results of numerical calculations and their comparison with the full-scale examination are provided in the paper. A general tendency to overestimate the permeability persists. It may be associated with the application of a rather crude resistive model for assessing permeability and neglecting taking into account the porous cement.

2

2 Method

Simulation of the rock cores pore space is carried out in several stages. Primitives of the shapes of grains, granulometric composition, and rock texture are modeled during the first stage. The coefficients of filling the pore space with clay cement are given. The parameters of the physical model, the calibration algorithm, and the presentation of the results are indicated at the last stage. As a result, a model of porous medium is designed. The obtained model is used for modeling of filtration processes in porous formation environment.

A developed digital rock model consists of several embedded models:

- rock microstructure model
- numerical permeability models and filtration-capacitance rock properties
- numerical models of asphaltene, paraffin and resin precipitation.

The first one is the construction of the 3D geometry of the rock microstructure, the second one is the simulation of micro-flow physics, and the third one is chemistry of processes occurring under reservoir conditions. These components are integrated into a single digital rock model, designed to provide a means of predicting behavior of fluids under different conditions. This report examines the approaches to constructing the geometry of the microstructure of a rock.

A rock microstructure model obtained by the stochastic[6-8] or simulated packing algorithm of microparticles with compaction is used as a basis for the subsequent analysis of pore space. Having made the transition from the representation of particle packing to the representation of the pore network model, the permeability of single channels can be calculated using molecular dynamics. Thus, for the network model of the pore collectors, a system of linear equations is compiled with respect to the pressure in each pore. The evaluation of a sample pressure drop makes it possible to calculate the absolute permeability according to Darcy's law[9].

In the report we have suggested a simplified model of the geometric structure of rock core space, i.e. a box densely filled with some balls of different diameters. The distribution of the diameter of the balls can be obtained by the laboratory studies of the rock core (Fig. 1). Packing of balls is made as a result of simulation of molecular dynamics. The box has fixed walls and bottom. Simulation of molecular dynamics has been done with atoms having the radius of the van der Waals interaction corresponded to the distribution, determined as a result of laboratory rock core studies (Fig. 1).

The Lennard-Jones (LJ) potential (1) is chosen as an interatomic interaction potential because of its simplicity and because it has never led to physically unacceptable results. It can be applied to model not only atoms and molecules with spherical symmetry but also other non-polar substances:

$$U(r)=4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right] \quad (1)$$

where ϵ is the depth of the potential well, σ is the finite distance at which the inter-particle potential is zero, r is the distance between the particles.

The parameters σ are used according to the radius of a corresponding ball, and the cross-section interaction parameters have been defined using the Lorentz-Berthelot mixing rule (2):

$$\epsilon_{ij} = (\epsilon_{ii}\epsilon_{jj})^{\frac{1}{2}}, \sigma_{ij} = \frac{1}{2}(\sigma_{ii} + \sigma_{jj}) \quad (2)$$

Gravitational force has also been applied. To save computing time the LJ potential has been truncated at a cut-off distance of and to avoid a jump discontinuity at cut-off distance, the LJ potential has been shifted. During the simulation the temperature linearly decreases passing the melting point down to the low values. For the temperature maintenance the Berendsen thermostat have been used.

Passing the coordinate space of the box with a specific test atom having specified van der Waals radius is sufficient to determine the pore space. The result is a system of micro-channels, which can be used within the electrodynamic analogy, presenting trends in the form of a network-related electrical resistances. Having solved the problem of finding the impedance, one can found permeability.

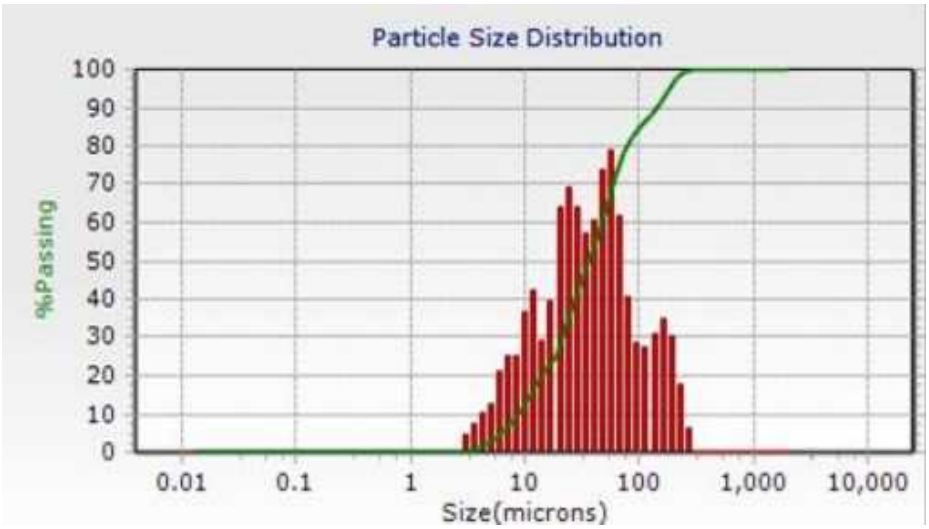

Fig. 1. The bar graph shows the percentage distribution of the particle size of the core sample. A graph of the cumulative volume is shown by the green line. The value of cumulative data is the percentage of particles whose size is less than the specified. The graph of the cumulative volume with the axis"% Passing" (% of the recorded data) and the axis "Size (microns)" is displayed on a semilogarithmic scale. Table 1 shows the results of an experimental study of the core sample and a numerical experiments with the fitted model.

4

3 Computing Details

The NArFU Computing cluster [11] with a peak performance of 17.6 TFLOPS, has a hybrid architecture consisting of twenty 10-core dual-processor nodes with an Intel Xeon processor, eight of which have Intel Xeon Phi coprocessors. The nodes are connected by the high-performance interconnect Infiniband 56. The computing cluster has the following characteristics:

- 20 computing nodes.
- Each node has two 10-core Intel Xeon E5-2680v2(2,8 GHz) processors and 64 GB of RAM.
- At eight nodes, the Intel Xeon Phi 5110P (8GB, 1.053 GHz, 60 core) math coprocessors are additionally installed.
- Internal computer network for calculations: Infiniband 56 Gb / s.
- Network file system FEFS (Fujitsu Exabyte File System) with a capacity of more than 50 TB and a throughput of 1.67 GB / s (13.36 Gb / s).
- The cluster performance on the CPU in the LINPACK test is 8.02 Tflops; on the CPU + Xeon Phi 7.68 Tflops, the cumulative 15.7 Tflops.

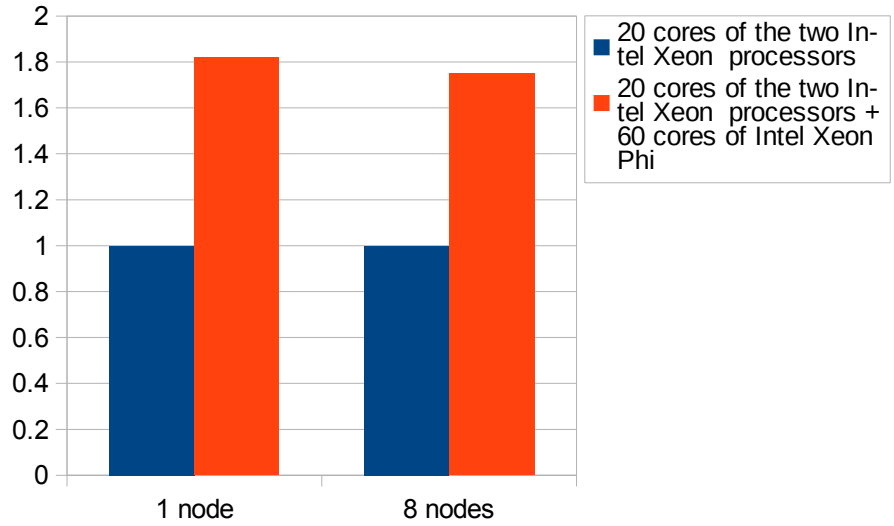

Fig. 2. Acceleration with the Intel® Xeon Phi ™ coprocessor in offload LAMMPS numerical simulation

The modeling of the geometric structure of the rock core space have been carried out-out using molecular dynamics methods, using the application software package LAMMPS[12]. LAMMPS parallel simulator of atomic, meso or continuous scale atomic models. It can be executed both on one processor system, and using the technique of message passing (MPI) with the help of spatial partitioning of the calculation area. Since 2015, the support for the using of Intel® Xeon Phi ™ coprocessors has

appeared as a part of the code being redistributed to date. A number of LAMMPS routines are optimized for operation in the offload mode of the Xeon Phi ™ operation. The comparison of computational performance with and without applying a coprocessor is illustrated in Fig.2.

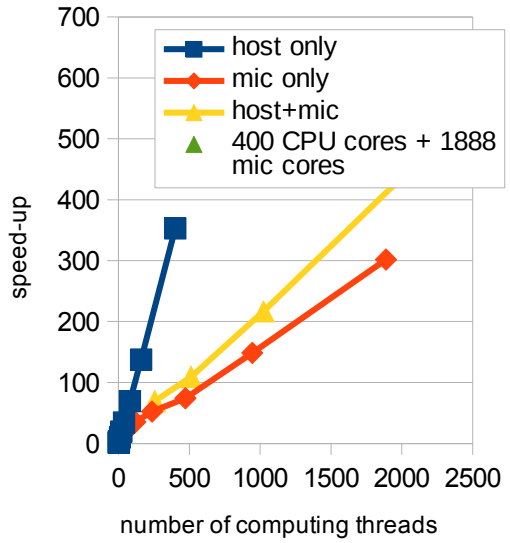

Fig. 3. Host only, mic only, host+mic and overall cluster speed-up versus number of computing threads for dedicated case code for molecular dynamics creation of rock microstructure

Due to the fact that the accuracy in calculating the step motion is not so demanding to simulate molecular dynamics for creating the rock microstructure geometry, the calculation can be performed with a single precision. This was used in the development of dedicated custom code[13] for constructing the geometry of a microstructure using molecular dynamics. As a basis, the code for solving the N-body problem has been taken from [14] and an appropriate optimization has been carried out, containing scalar tuning, vectorization with SoA and memory optimization. OpenMP threads on the coprocessor have been started started in offload mode. Data between nodes have been synchronized with MPI processes running on CPU nodes. Such an approach has yielded approximately 12 times the performance in comparison with LAMMPS. Scaling properties of code are shown in Fig. 3.

4 Core Samples Investigation

The experimental studies of the terrigenous reservoir, represented by a single core sample of standard size 30 mm in diameter and 30 mm in length, have been carried out. The coefficient of open porosity have been determined on the sample by the method of liquid saturation in accordance with (GOST 26450.1-85. The method of determining the coefficient of open porosity by liquid saturation) and the coefficient

of absolute permeability in accordance with (GOST 26450.2-85. Gas permeability for stationary and non-stationary filtration.) Residual water saturation - by capillarimetry method in accordance with GOST 39-204-86 Oil Method for determination of residual water saturation pit oil and gas.). After that, the sample has been saturated with kerosene and the core permeability has been determined by fluid in the formation conditions at the PEC-5 (7) installation.

Table 1. Results of natural and numerical investigations

	Connected porosity, %	Permeability for kerosene, 10^{-3} um^2
Natural rock core samples	20.11	55.66
Stochastic packing	25.82	68.45
Molecular dynamics simulation packing	22.27	60.92

After carrying out the filtration experiments, the input end of the sample have been photographed, and subsequently have been cut by 1 mm along the length of the sample by grinding and again photographed. The operation have been carried out to the full "attrition" of the sample. In the course of these experiments an array of image layers has been obtained, which can be used in the validation of a digital model of the rock microstructure. It is important to determine the granulometric composition of sandy-silty rocks to study out their properties as oil and gas collectors[10]. Determination of the granulometric composition of the sample has shown that the average particle diameter by the type of distribution of their number is 5.82 um, the average particle diameter by the form of their distribution is 54.52 um. The obtained percentage distribution of the particle size of the core sample is shown on Fig.1. Table 1 shows a comparison of the results obtained by the methods described above.

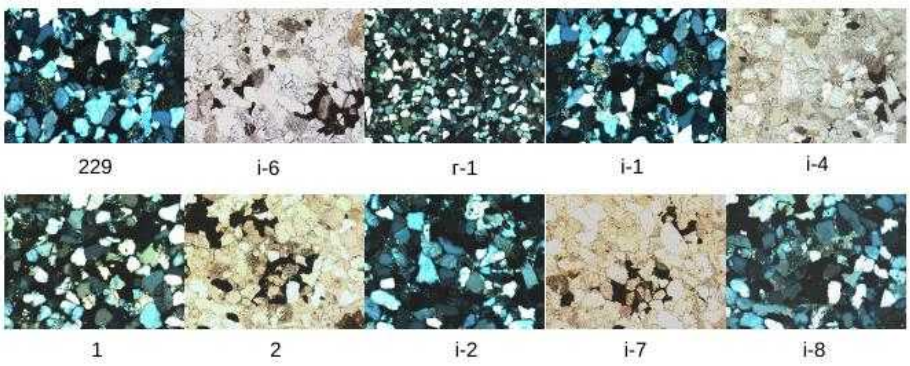

Fig. 4. Photos of the sections of core samples. 100x magnification. Polarized light for 229, r-1, i-1, 1, i-2, i-8. and passing light for i-6, i-4, 2, i-7.

Petrographic description of 10 thin sections (Fig. 4) of the terrigenous sandstone rocks of Berea Sandstone field has been performed to obtain lithological and petrographic information. The investigated samples are medium-fine-grained and finely-medium-grained light-gray sandstones which are the reservoirs with mainly average usable storage capacity pore-type. Their porosity according to petrophysical analyzes varies in the range of 17-20%. In terms of material composition: the content of quartz in rocks varies within the limits of 70-85%, feldspars 2-5%, fragments of rocks of different genesis of 10-20%, mica 1-2%. Cement mixed: locally developed cementation of contact type with conformal contacts of individuals; regenerative quartz does not exceed 1%; pore-film cement clay 2-5%; Authigenic carbonate plays the role of porous corrosive cement (2-5%). The key factor determining the porosity and permeability of terrigenous reservoirs is the dimension of the grains of rock-forming minerals and their sorting. A direct relationship between the grain size and the porosity of the rocks along the sections has been shown in natural and simulated examinations. The larger the grain size, the greater the porosity. It should also be emphasized that in these rocks quartz grains and rock fragments have an irregular shape and semi-entangled particles, thus they are laid less densely, which leads to an increase in porosity.

Table 2. Open porosity and absolute permeability of investigated core samples.

Sample	Length, cm	Diameter, cm	Absolute permeability, 10^{-3} um^2	Open porosity, %
r-1	3,068	3,003	101,01	20,11
i6	2,682	2,997	125,64	20,42
i1	3,110	2,999	130,25	17,99
i2	2,722	2,996	96,43	18,89
i4	2,743	3,002	85,82	17,48
i7	2,854	3,003	91,64	18,55
229	2,974	2,995	121,13	19,63
1	3,580	2,995	101,032	18,07
i8	2,967	2,997	97,22	18,52
2	3,630	3,003	83,64	18,79

A dependence of permeability on the temperature of the rocks (Table 2, Fig. 5) has been shown in natural and simulated examinations. The graphs obtained during examinations of the permeability of ten samples are presented. Two graphs of permeability calculated for two simulated microstructures and comparison are also presented: the first one is for the microstructure obtained by stochastic packing, the second one is for the microstructure from molecular dynamics simulations. The permeability coefficient of clastic rocks is affected by: the granulometric composition of the rocks, sorting, the shape of the grains and packaging. A comparatively close direct relationship between permeability and granulometric composition is established in the investigated terrigenous rocks (Fig. 6). The correlation coefficient R is 0.467. The composition and content of the cementitious material is also reflected on the reservoir properties.

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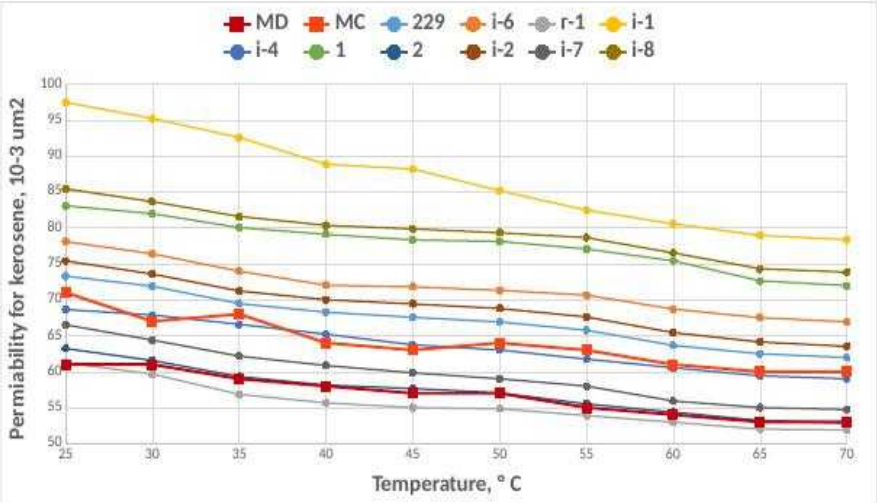

Fig. 5. Natural and numerical core sample investigation of permeability dependence from the temperature. Circles indicates data from natural experiments. Square indicates data from simulations. MD for molecular dynamics and MC for stochastic packing.

The characteristics of the rock surface, depending on the wettability have been investigated. In general, for all samples, the wettability index varies within the range 0.03-0.94, the average value of 0.55, the rocks of the samples studied can be characterized as hydrophilic and as hydrophobic. Surface properties of rocks are one of the most important characteristics, they affect the distribution of fluids in the pore space and largely determine the process of oil recovery. It is not possible to evaluate unambiguously the wettability of terrigenous rocks having a complex pore space structure, a heterogeneous mineralogical composition. Most researchers are of the opinion that the surface of carbonate rocks has heterogeneous wetting properties, that is, hydrophilic and hydrophobic regions coexist simultaneously. The research of this collection has supported it. Wettability of rocks is determined by the material that makes up the rock, but can change under the action of the liquids contained in the pores, that is, it depends on the properties of oil and water. It is known that in the formation oil there are surface-active and polar substances that can be adsorbed by the rock. Therefore, the integral wettability of rocks is a complex function that depends on the properties of the rock and liquids that saturate the pore space(Fig. 7).

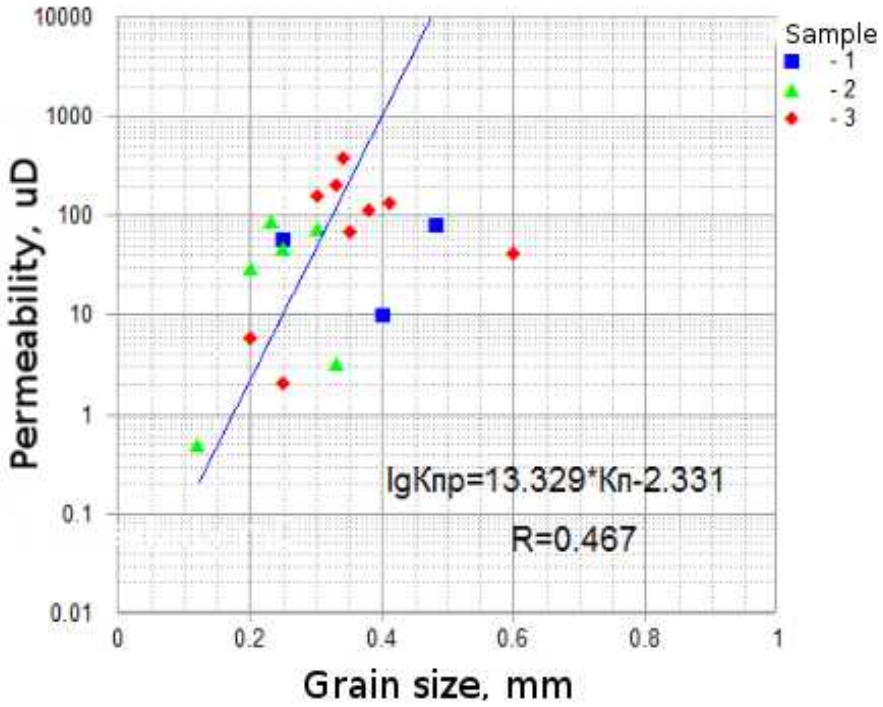

Fig. 6. Dependence of permeability on average grain diameter for core samples from different deposits

According to the graph, there is no clear correlation between the core permeability for oil and the wettability index. Both hydrophilic samples and hydrophobic samples are present and have a permeability coefficient from 10^{-3} μm^2 to 10^{-1} μm^2. The question of how the wettability of the collector surface changes when it is saturated with oil has not been clarified at the present time. In this connection, the hydrophobic ability of oil in contact with the surface of reservoir rocks is an object of interest.

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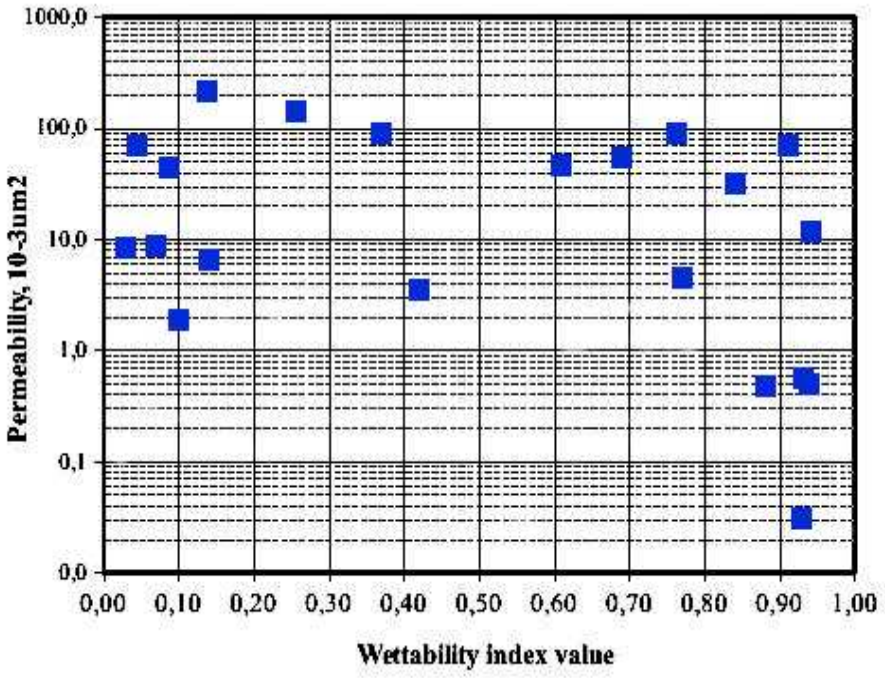

Fig. 7. Comparison of permeability and wettability index

5 Conclusions

An approach to the solution of the problem of mathematical modeling of macroscopic properties of porous media is proposed in which the molecular dynamics method is applied for 3D reconstruction of the rock microstructure. The results of numerical calculations and their comparison with the full-scale experiments are presented. There is a general tendency to overestimate the permeability, which may be associated with the usage of a fairly coarse resistive model to assess permeability and the fact that porous cement is not taken into account.

Acknowledgements

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