Digital core modeling technology for determining the reservoir-capacitive properties of terrigenous reservoirs

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Abstract. For today digital core modelling technology is demanded and developing instrument in conducting the main reservoir-capacitive properties of terrigenous rocks. This technology is becoming more widespread in connection with the development of computer and nanotechnologies. The main attempts to apply the digital core model in practice have been undertaken in the last decade, although the first examples of its use for the analysis of reservoir rocks date back to the 80s of the last century. Improvement of digital core modeling technology will allow to cope with the problem of lack or absence of core material, as well as to solve the problems of studying loose, weakly cemented and other rocks, "problematic" of conducting physical experiments. In addition, it seems relevant to create a digital core block that fits into the general digitalization platform of technologies related to reservoir-capacitive properties in the development of hydrocarbon fields. With the use of a digital core model, it also becomes possible to effectively refine and supplement the calculated parameters in laboratory core studies, reducing the likelihood of errors in the obtained results.

1. Introduction
Currently, digital core modeling technology is a popular and developing area in the assessment of geological oil reserves in the World [1 - 8]. The issue of digital core modeling seems to be relevant due to the fact that specialists do not always have a sufficient amount of core material from wells to conduct research, in some cases it is not possible to select core material [9]. For example, in cases where the core from the investigated wells is represented by loose, weakly cemented and other rocks. Sometimes the core from the studied wells is completely absent. In this regard, specialists of core laboratories often have to limit themselves to an insufficient amount of core material to determine the desired characteristics of the formation. At the same time, when there is no core material from the wells of interest at all, one has to restrict oneself to the data of geophysical studies of wells and the results of other studies.

With the help of a digital core model, it also becomes possible to effectively refine and supplement the calculated parameters obtained in the process of laboratory core studies, thus reducing the likelihood of errors in the results. So, after conducting experiments to determine the permeability of the core when modeling reservoir conditions, a specialist will be able to check the result obtained by mathematical modeling in a digital core model on a supercomputer. In the event of serious contradictions in the results between laboratory experiments and mathematical modeling, a decision may be made to repeat the physical experiment or to cancel it. All this allows to talk about digital core
modeling as an effective and relevant additional tool that is necessary to increase the validity of the results of laboratory core studies.

2. Selection of the main parameters of terrigenous oil reservoirs for the formation of a digital core model

Terrigenous sediments are clastic sediments and detrital rocks, consisting of fragments of rocks and mineral grains taken from the ground. Terrigenous rocks include sandstones, siltstones and other rocks. Terrigenous rocks are among the most common reservoirs of oil and gas. According to various estimates, up to 80% of oil reservoirs are confined to them [10]. The study of terrigenous rocks is an important issue in the study of oil and gas reservoirs.

Pores and pore channels in terrigenous rocks form a complex structure of pore space through which oil migrates from the reservoir to the bottom of the well. Pore channels are complex capillary systems and locate in terrigenous rocks in a chaotic manner, have different sizes, shapes, directions, physical and chemical composition of rock grains and cement that make up the rock matrix. It should also be noted that not all pores and pore channels of terrigenous rocks are opened and communicating. Some of them are closed and do not participate in the processes of oil migration.

Thus, it can be noted that even a standard-size terrigenous core sample of rock with a diameter of 30 millimetres and a length of 30 millimetres in its volume can have a huge number of pore channels, in which a large number of factors occur. These factors include the geometry of the pore channels, reservoir and rock pressure, reservoir temperature, capillary pressure, which prevents fluid displacement, and many other factors.

The reservoir-capacitive properties of rocks are determined by porosity and permeability, as well as their material composition. Reservoir properties are one of the most important parameters of terrigenous oil reservoirs. The range of permeability of terrigenous oil reservoirs is wide and can vary from less than 0.0001 $\mu$m$^2$ to several $\mu$m$^2$, depending on the rock type and other factors. The coefficient of open porosity of terrigenous rocks is also within wide limits and can vary from fractions of a percent to 50 and more percent.

At the initial stage of the formation of a digital core model, methods should be used with the help of which it is possible to determine the shape and size of the grains that make up the rock. Subsequently, a model of a porous medium is formed from the modeled grains, into which various processes and parameters are embedded. These methods include the determination of the particle size distribution using laser diffraction analyzers, microtomography of rocks, and studies of petrographic thin sections. To understand the volumetric characteristics of the pore space of the rock, it is important to determine the coefficients of opened, effective and dynamic porosity of the rocks. Microtomography of rock samples can be used to study the structure of the pore space, assess the effective porosity, and the nature of water saturation, even in the absence of core material [11]. Tomographic studies - to assess lithological heterogeneity at the micro level, to obtain a three-dimensional model of the structure of the void space [12]. Depending on goals a specialist pursues in digital modelling, parameters that are important for determination may be the permeability of the rock to fluid or gas, phase permeabilities, residual water saturation, petrophysical parameters of rocks, and other characteristics.

3. Creation of digital core model structure

The proposed digital model of the core is a dense stochastic packing, which composes its microstructure, for the creation of which molecular dynamics methods can be used.

When using dense stochastic packing, the core particles in the digital model are initially represented by spheres, the size of which is selected based on the data obtained during the determination of the particle size distribution of the samples, microtomography or the results of lithological and petrographic studies of thin sections. However, it should be borne in mind that rock particles are not homogeneous in their physical and geometric properties, and rarely have a shape that is close to the shape of a sphere. This is confirmed by a number of works, including [13]. Particles of
Terrigenous rocks can have cubic, prismatic, tabular and other structures, characterized by the degree of roundness and other geometric parameters. All this makes the stochastic packing of the digital core model, consisting of spheres, ineffective and forces researchers to form a packing of figures of a different geometric shape, such as spherocylinders, spherocubes and spherocubes [14].

In the process of using a dense stochastic packing of the proposed digital core model, the centers of growth of the spheres are initially randomly scattered in the volume, after which they grow until they collide with neighbouring ones, then the distribution of the position of the spheres corresponding to the given one occurs. Then, the transition from spheres to more complex geometric shapes can be done.

In the process of generating a dense stochastic packing for modeling the rock structure based on the distribution of the grain sizes of rocks, the Monte Carlo method can be applied. In this case, the sizes and other parameters of the grains can be determined from the images of thin sections, according to the granulometric analysis of rocks by laser diffraction or other methods. In the future, when forming a digital model, molecular dynamics methods can be used.

The model of the microstructure of the core obtained using the stochastic packing of microparticles with compaction can be used as a basis for the subsequent analysis of the pore space. After the transition from particle packing to the pore network model, the conductivity of single channels is calculated using molecular dynamics; To estimate the absolute permeability of the modeled microstructure, an electrohydrodynamic analogy can be used in the future, while the mass conservation law is fulfilled for each uninsulated pore (open porosity); thus, for the network model of the pore space, a system of linear equations for the pressure in each pore is compiled [15]. The estimation of the pressure drop across the sample makes it possible to calculate the absolute permeability according to Darcy’s law [15]. The finite volume method can also be used to numerically simulate gas and fluid flows on a macroscopic scale. The implementation of this method should be adapted for multiphase systems, and the algorithm should allow achieving high accuracy of the pressure field.

In the proposed digital core model, the adsorption of substances in its microstructure can be investigated using the Monte Carlo method in a rigid, that is, with stationary particles, core model. In this case, the chemical potential is used as the input parameter of the model, and not the pressure, therefore, to determine the pressure of the adsorbed substance at a certain chemical potential, a special simulation of the Monte Carlo method is used for one reservoir in an isobaric-isothermal ensemble. The molecular dynamics calculation is started from the equilibrium configuration obtained using Monte Carlo simulations, and then the model is brought to an equilibrium state. The speed Verlet algorithm is used to integrate the equations of motion. The temperature of the model is controlled by a Berendson or Noise-Hoover thermostat. From molecular dynamics simulations, by calculating the root mean square displacement using the Einstein equation, diffuse values are obtained for the required conditions. To describe the properties of the filtration flow, the root-mean-square deviation of the center of mass of particles in the model is calculated, which corresponds to the corrected diffuseness or diffuseness of Maxwell-Stefan. The obtained diffusion coefficients are further used to estimate the conductivity of single channels of the digital core model using the Knudsen model.

Thus, the issues of creating and improving the digital core modeling technology lead to the need for multiscale modeling and finding solutions to a number of problems. In practice, each of the above methods is implemented in one, or more often, several software packages that have a similar scope of application, but often these packages involve the use of different algorithms and approaches to solving problems, their implementation is different. When carrying out complex studies, such as those described in the above example, it is necessary to organize the sequential operation of various software packages, so that the result of the work of one package is submitted as input for the next one. It should be noted that there are no universal standards for input and output data formats for this kind of research, and as a result, specialists need to constantly correct data in the interval from the output of one computational package to the input for another. In some cases, this problem can be solved by
using additional software that is necessary for converting formats, or simply converting some data structures to others, but, nevertheless, there are no universal tools applicable to this task today.

Automation of the construction of workflows, when with the help of middleware, the sequential execution of tasks by the necessary software packages and the transfer of data from one package to another is organized, would significantly reduce the time required for conducting computational experiments. Such automation will also allow avoiding errors that can appear if the data is incorrectly transferred and entered by specialists.

One of the possible approaches to integrating heterogeneous software is to organize interaction through a single repository, when the result of the work of any software package will be converted into some common format, stored in the repository, and, subsequently, the necessary data for launch the next package will be retrieved from the repository by converting from the common format to the input of the next software product in the workflow.

This approach also allows for the implementation of the concept of "collective intelligence". This approach can be of great importance, taking into account the fact that many tasks of digital core modeling require significant computational resources and run computational packages on high-performance computing systems.

4. Results and discussion
In the work, studies were carried out to determine the calculated permeability with a change in temperature with respect to kerosene on a digital core model. The calculated permeability was determined for two structures. The first structure was a dense stochastic packing of microparticles, the second was a core microstructure modeled by the molecular dynamics method.

As a result of modeling the microstructure of the core, a system of microchannels was built, in which the method of electrodynamic analogy was applied to determine the permeability. The process of fluid movement in the model was "replaced" by the process of current flow through a circuit with resistance and, accordingly, the problem of finding the rock permeability in the network of microchannels of the porous medium was "replaced" by the problem of finding the current strength in the electric circuit. Filtration flows were presented through a network of connected electrical resistances. Having solved the problem of finding the impedance, the total calculated permeability of the model can be determined.

Based on the simulation results, the dependence of the permeability of the digital core model on temperature was obtained (Figure 1). Similar dependences were obtained from the results of laboratory studies of physical core samples (Figure 2). The results obtained showed good convergence. As can be seen from the graphs, the curves of the change in permeability versus temperature obtained during studies on physical samples and a digital model have a similar character and is in the same range.
In the course of the work, studies were also carried out to create digital models of the core for the terrigenous reservoir rocks from the Timan-Pechora oil province with further determination of opened porosity and absolute permeability from them. The same experiments were carried out on physical samples in accordance with Russian regulations. The results showed good convergence. The average deviation in determining of opened porosity for 4 samples was 5.48%. The average deviation in determining of absolute permeability was 12.53%. The results are presented in the Table 1.
Table 1. The results of opened porosity and absolute permeability determination for the terrigenous reservoir rocks from Timan-Pechora oil province with use of digital core model

| № of sample | Absolute permeability, $10^{-3}$ micrometer$^2$ | Calculated absolute permeability (digital core model), $10^{-3}$ micrometer$^2$ | Deviation $\Delta K$, % | Opened porosity, % | Calculated opened porosity (digital core model), % | Deviation $\Delta K$, % |
|-------------|-----------------------------------------------|-------------------------------------------------|------------------|-----------------|-----------------------------------------------|------------------|
| 1           | 48.91                                         | 54.90                                           | 12.25            | 16.10           | 16.82                                         | 4.28             |
| 2           | 9.29                                          | 10.61                                           | 12.44            | 8.30            | 8.84                                         | 6.11             |
| 3           | 59.30                                         | 70.34                                           | 15.92            | 18.40           | 18.96                                         | 2.95             |
| 4           | 84.01                                         | 93.22                                           | 9.51             | 18.60           | 20.35                                         | 8.60             |

5 Conclusion
In this work the technology for determination the filtration-capacity properties of terrigenous reservoirs on a digital core model has been substantiated, which allows obtaining representative results using mathematical modelling methods.

Based on a comparison of the results of determining opened porosity, absolute permeability and permeability by kerosene on a digital model and data from laboratory studies on core material, it is shown that the introduction of digital modelling makes it possible to increase the efficiency of simulating filtration processes in reservoir conditions of the studied objects, and it seems expedient to use it in carrying out activities related to geological information support for the commissioning of hydrocarbon reservoirs.

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