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MINING ROCK PROPERTIES. ROCK MECHANICS AND GEOPHYSICS

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Formation of synthetic structures and textures of rocks when simulating in COMSOL Multiphysics

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Abstract
Rock texture and structure play an important role in the formation of the rock physical properties, and also carry information about their genesis. The paper deals with the simulation of geometric shapes of various structures and textures of rocks by the finite-element method (FEM). It is carried out by programmed detailing of the element properties and their spatial location in the simulated object. When programming structures, it is also possible to set the physical properties of various parts of the model, grids, initial and boundary conditions, which can be changed in accordance with the scenarios for numerical experiments. In this study, on the basis of FEM, simulation of various structures and textures of rocks with inclusions and disruptions was implemented in COMSOL Multiphysics in conjunction with Matlab. Such structures are used to conduct computer generated simulations to determine physical properties of geomaterials and study the effect on them of agents of various physical nature. The building of several models was considered: a rock specimen with inclusions in the form of ellipses of equal dimensions with different orientations; a sandstone specimen containing inclusions with high modulus of elasticity in cement matrix when deforming; a limestone specimen with fractures filled with oil and saline water when determining its specific electrical resistance. As an example of a fractured structure analysis, the influence of the filler on the electrical resistance of the limestone specimen containing a system of thin elliptical predominantly horizontal fractures was considered. The change in the lines of current flow at different ratios between the matrix and the fracture filler conductivities and their effect on the effective (averaged) conductivity of the rock specimen was clearly demonstrated. The lower conductivity of the fracture filler leads to increasing the length and decreasing the cross-section of the current flow lines that, in turn, leads to significant decrease in the conductivity of the fractured rock specimen. The higher filler conductivity results in a slight increase in the conductivity of the fractured specimen compared to that of the homogeneous isotropic specimen. The resulting structures can be used for numerical experiments to study physical properties of rocks.

Key words
rocks, geomaterials, physical properties, fractures, inclusions, numerical simulation, synthetic structures, texture, acoustic properties, electrical properties

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СВОЙСТВА ГОРНЫХ ПОРОД. ГЕОМЕХАНИКА И ГЕОФИЗИКА

Научная статья

Формирование синтетических структур и текстур горных пород при их моделировании в среде COMSOL Multiphysics

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Аннотация
Текстура и структура горных пород играют существенную роль в формировании их физических свойств, а также несут информацию о генезисе. В статье рассматривается моделирование методом конечных элементов (МКЭ) геометрических форм различных структур и текстур горных пород. Оно осуществляется путем программной детализации свойств элементов и их пространственного расположения в моделируемом объекте. При программировании структур возможно также задание физических

свойств различных частей модели, сеток, начальных и граничных условий, которые могут изменяться в соответствии со сценариями проведения численных экспериментов. В работе на основе МКЭ реализуется моделирование в COMSOL Multiphysics в связке с Matlab различных структур и текстур горных пород с включениями и нарушениями. Такие структуры используются для проведения компьютерных экспериментов по определению физических свойств геоматериалов и исследованию влияния на них воздействий различной физической природы. Рассмотрены построения нескольких моделей: образца горной породы с включениями в форме эллипсов равных размеров с различной ориентацией; образца песчаника, содержащего включения с высоким модулем упругости в цементирующей матрице при его деформировании; образца известняка при определении его удельного электрического сопротивления с трещинами, заполненными нефтью и минерализованной водой. В качестве примера анализа трещиноватой структуры рассмотрено влияние заполнителя на электросопротивление образца известняка, содержащего систему тонких эллиптических трещин с преимущественно горизонтальным расположением. Наглядно показано изменение линий протекания тока при разных соотношениях между проводимостью матрицы и заполнителем трещин и их влияние на эффективную (усредненную) проводимость образца породы. Меньшая проводимость заполнителя трещин приводит к увеличению длины и уменьшению сечения линий протекания тока, что в свою очередь приводит к существенному снижению проводимости трещиноватого образца породы. Большая проводимость заполнителя имеет своим результатом незначительное увеличение проводимости трещиноватого образца по сравнению с однородным изотропным образцом. Полученные структуры могут быть использованы для проведения численных экспериментов по исследованию физических свойств пород.

Ключевые слова

горные породы, геоматериалы, физические свойства, трещины, включения, численное моделирование, синтетические структуры, текстура, акустические свойства, электрические свойства

Финансирование

Работа выполнена при финансовой поддержке гранта РФФИ (проект № 20-05-00341)

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Introduction

Rock texture and structure play an important role in the formation of a rock's physical properties and also carry information about their genesis. Therefore, scientists from different disciplines have an interest in studying these rock characteristics.

The history of the evolution of texture analysis (TA) was presented in the fundamental study by [1], which gave examples simulating the elastic properties of textured materials from multiphase specimens containing pores and fractures. Petrographic analysis was carried out by [2] to determine the structure, texture, composition, and presence of minerals in beach rock specimens from the islands of Japan and Indonesia. To optimise the parameters of hydraulic fracturing using two and three-dimensional numerical models, the matrix structure and heterogeneities of minerals with complicated geometry of intergranular contacts between them were taken into account [3]. The importance of studying texture as one of the key elements that determine the morphological features of rupture was noted in [4]. Studies of small-scale variations in mineralogical composition and texture associated with rock faults within the San Andreas continental transform fault zone were described in [5]. Crystallographic textures of specimens of granulite, amphibolite, schist and gneiss were measured, classified, and compared with similar textures of monomineral rocks in [6]. In [7], analysis of the crystal structure, texture, and chemical composition of synkinematic phyllosilicates in fault zones was used to determine the mechanisms and stages of strains and conditions of fault activity. Replacing the models of the complex textures of most granular sedimentary rocks with a model of a granular effective medium, based on the physics of random sphere packing, was proposed in [8]. The physical properties of reservoir rocks containing oil, gas, or water depend on the rock mineral composition and texture, as noted in [9]. The texture and residual stresses in geological specimens were studied in [10]. The theory and simulation of the formation of new structures as a result of the contrast in rheological properties between layers of different textures were considered in [11].

A number of studies have been devoted to the quantitative assessment of textures using coefficients, as well as the establishment of their relationship with the physical and technological properties of rocks.

The texture coefficient was proposed by two Australian researchers, Howarth and Rowlands, in 1986 [12, 13] to quantify texture, taking into account the shape, size, and location of mineral grains that made up rocks, as noted in [14]. The relationship between a rock's engineering properties and texture has been investigated through examples of carbonate rocks [15]. Grain shape, elongation, orientation, roundness, packing density, porosity and matrix content were evaluated by the texture coefficient.

Specimens of Cretaceous carbonates, including grain size and percentage, matrix type, dolomite percentage and carbonate percentage were investigated in relation to compressive strength and Young's modulus [16]. Quantitative petrographic studies of the influence of the distribution of minerals and their sizes on the strength and other geotechnical properties of low-porosity volcanic rocks were discussed in [17]. The relationship between the texture coefficient and sinuosity of the matrix of a rock containing pores (on the one hand) and Young's modulus, ultimate strength, ultimate yield and shear modulus under uniaxial compression (on the other), was investigated in [18]. Experimental numerical simulation by the method of discrete elements and laboratory testing of granite specimens under uniaxial compression and Brazilian tests (for tensile strength) were performed in [19], to study the effect of the size and distribution of mineral grains on the strength and nature of microfractures in granite rocks. The influence of the pre-existing texture of natural fractures on the shape of the reservoir in the course of its hydraulic fracturing was studied in [20] using a block model of discrete elements. The influence of the mineral composition and texture of the rock on the slake durability index (Slake Durability, SDI), as well as the relationship between the SDI of some rocks and their engineering (geotechnical) properties were studied in [21]. The relationship between the texture and mechanical properties of various rocks was studied in [22]. The rock texture features were quantified using the texture coefficient. The developed model was applied to determine the rating of intact rock mass in the RMR rock mass classification.

A special place is occupied by methods of image processing and synthesis of structures to establish their relationships with the physical properties of rocks.

The study [23] was devoted to the automatic identification of rocks in thin sections using texture analysis. The publication [24] is devoted to the creation of petrographic images using thin sections and the quantitative determination of the spatial location of selected rock components using two-dimensional (2D) Fourier transform. The texture segmentation algorithm for digital images of borehole walls was discussed, based on the "texture energy" index, and allowed to automatically divide the recorded sequence into strata [25]. The use of the statistical texture model proposed by Ma and Gagalovich to create a synthetic image comparable to the original one, was described in [26]. The study by [27] was devoted to the automatic identification of rocks in thin sections using texture analysis. Stress-strain curves and rupture evolution processes in rocks, based on synthetic digital models under uniaxial compression that allowed the simulation of various structural details and heterogeneous diversity of the studied rocks, were studied in [28]. The pore network model was used in [29], to simulate diagenetic cycles of sedimentary reservoir rocks. An example of the use of two extended fracture criteria - the “nonlocal Coulomb-Mohr softening criterion” and the “multilayer criterion” - for simulating underground constructions and rock specimens in layered mica schist with overlying rocks of complex texture, was given in [30]. The textures of three different facies of diabase alteration were studied using microscopy and X-ray microtomography to calculate rock permeability by numerical simulation [31].

For the numerical simulation of various structures and textures of rocks with inclusions and fractures by the finite-element method in the COMSOL Multiphysics environment, the use of this software in conjunction with Matlab, on the basis of which this system was created, may be useful. The structures obtained in this way can then be used for carrying out computer generated simulations to determine physical properties of geomaterials and study the influences on them of the effects of diverse physical nature. The complexity and laboriousness of manually drawing such textures with a large number of structural elements, as well as with permanent changes in the course of performing a series of experiments, make this operation practically unfeasible.

The aim of the study was to develop a technology for the automated synthesis of structures and textures of rocks with random variations of given textural parameters, characteristic of natural geomaterials, for use in numerical experiments for determining the physical properties under diverse effects.

1. Research techniques

Finite-element simulation of geometric shapes of various structures and textures of rocks is carried out by means of drawing the elements and their placement within the simulated object using software. With this approach, it is also possible to set the physical properties of various parts of the model, grids, initial conditions and boundary conditions, which can change in accordance with the scenarios for conducting numerical experiments.

As an example of the formation of a structure created using a program written in Matlab codes, in COMSOL Multiphysics, we consider a fragment of a drawing of a rock specimen with inclusions in the form of ellipses [32]. The introduction of a random number generator makes it possible to obtain the uniqueness of each combination of geometric parameters and study the influence of random factors on the experiment results.

Code snippet

clc	Initial operations
clear all	
clear fem	

fem.shape = 2;	
fem.sshape = 2;	
AT = 0.001;	Semi-major axis of the ellipse
BT = 0.0002;	Semi-minor axis of the ellipse
phi = 45;	Ellipse tilt
LX = 0.032;	Specimen width
LY = 0.064;	Specimen height
NX = 15;	Ellipses horizontal quantity
NY = 18;	Ellipses vertical quantity
YMIN=BT/3;	Y fields
XMIN=AT/3;	X fields
DX = (LX-2*XMIN)/(NX+1);	Distance between inclusions along X
DY = (LY-2*YMIN)/(NY+1);	Distance between inclusions along Y
r1 = rect2(LX,LY,'base','corner','pos',[-LX/2 -LY/2]);	Specimen formation
for j=1:NX	
display=j	
CX = -LX/2+XMIN+DX*(j);	
for i=1:NY	
CY = -LY/2+YMIN+DY*(i);	
k = (i-1)*NX+j;	
A=pi/2*random('Uniform',-1,1,1,1)	Tilt angle of ellipses from −90° to +90°
r{k} = ellip2(AT,BT,'pos',[CX CY],'rot',A);	Formation of ellipses of inclusions
r1 = r1 – r{k};	Formation of structure
r1 = r1 + r{k};	
end;	
end;	
fem.geom =r1;	Structure building
display='femgeom'	
fem.mesh = meshinit(fem);	Grid formation
display='femmesh'	
fem.mesh = meshrefine(fem);	
display='meshrefine'	
figure, geomplot(fem)	Grid formation
fem.mesh = meshinit(fem,'report','off');	
fem.appl.mode = 'FlPlaneStrain';	Selection of a COMSOL Multiphysics section
fem.appl.equ.f = {0 0 1};	
fem.appl.equ.c = 1;	
fem.appl.bnd.h = 1;	
fem = multiphysics(fem);	
fem.xmesh = meshextend(fem);	
fem.sol = femlin(fem,'report','off');	
figure	
postplot(fem,'tridata','u')	Grid generation

This code corresponds to the generation of the structure in 2D space. Similarly, the generation in 3D space can be carried out.

2. The Findings and Discussion

2.1. Demo example

The result of generating the structure in accordance with the above code is shown in Fig. 1. In this case, the inclines of the ellipses were randomly set and their size and position did not change. By setting a different number of ellipses and changing their size boundaries, the incline angle and positions, it was possible to obtain structures corresponding to different types of rocks.

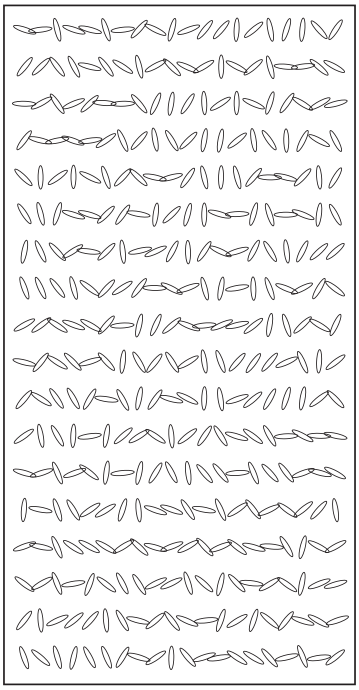


Fig. 1. The program code result

The resulting structures can be used for numerical experiments to study physical properties of rocks. We will now consider examples of such studies.

2.2. Generation of the structure of a sandstone specimen and simulating ts uniaxial compression test (UCT)

We will consider the simulation of a sandstone specimen of dimensions 32×32×64 mm in the form of a rectangular prism with a square base. The specimen included high-modulus grain-inclusions with a structure of 6×18 grains, placed in cement matrix. Semi-axes of the grains were of the following sizes: a large one of 1.8 to 2.9 mm and a smaller one of 1.3 to 2.1 mm. Orientation angles of the main axis of the ellipses were ±90° from the horizontal direction. The model's elastic properties, elastic modulus E and Poisson's ratio ν are given in Table 1.

Table 1

Elastic properties of the model elements

Structure elements	E, GPa	ν
Cement	1	0.2
Grains	100	0.25

In the simulation, the boundary conditions were set under which vertical displacements of the lower end were prohibited and the displacement of the upper end was 0.1 mm downward, corresponding to the vertical compression of the specimen.

The results of calculating the stresses in the specimen are shown in Fig. 2*a*; Fig. 2*b* shows the curve of vertical normal stresses in the $y = 0$ cross-section. In this case, it was assumed that negative values corresponded to the compressive stresses.

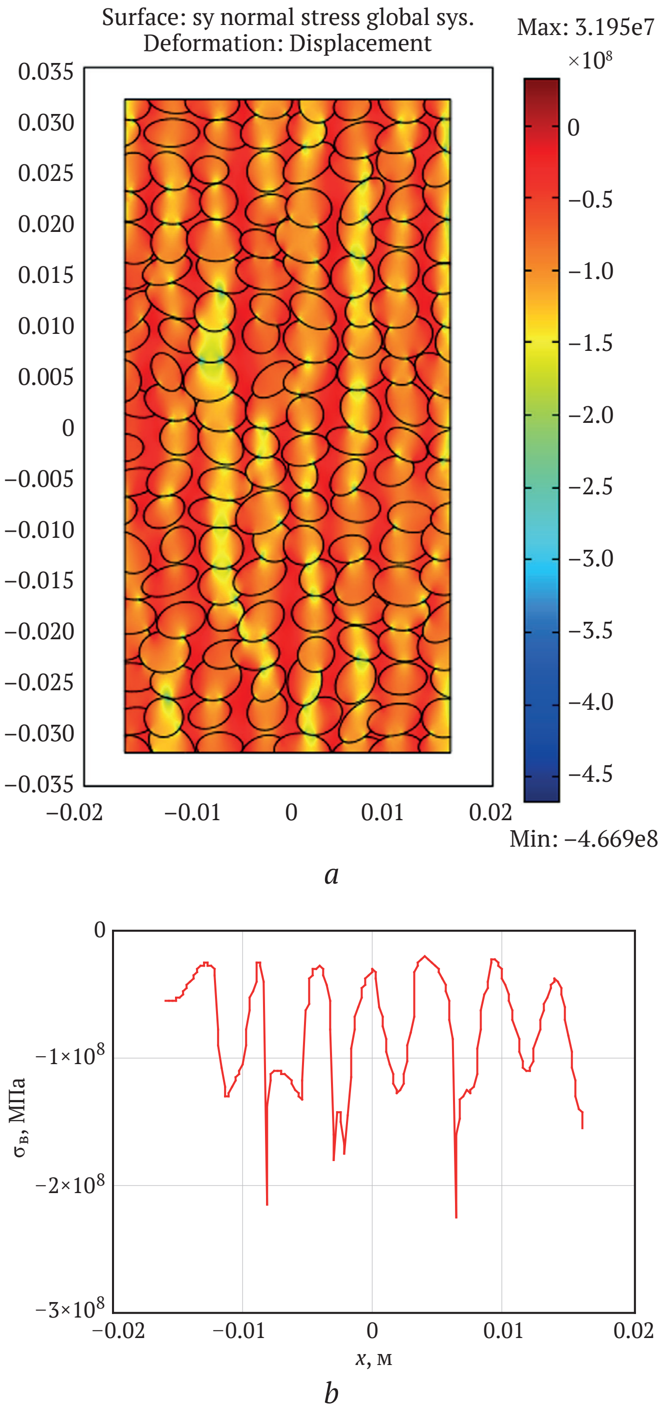


Fig. 2. The simulated structure of a sandstone specimen and distribution of vertical compressive stresses over the volume (*a*) and in the $y = 0$ cross-section (*b*) of the specimen

In Fig. 2*a*, the areas with the minimum compressive stresses (in absolute magnitude) are marked in red. The compression stresses at the grain contacts are marked in yellow, green, and blue. The areas of increased stresses, forming vertical chains, are marked in yellow. The maximum value of normal vertical stress in the $y = 0$ cross-section (in absolute magnitude) reached 223.8 MPa, and the average stress in this cross-section amounted to 77.0 MPa. The ratio of the maximum to average stress was 2.91. Large values of local stresses can cause destruction of the specimen's internal structure. If the specimen had a structure with a homogeneous modulus of elasticity, the compressive stresses averaged over the cross-section would not cause such a rupture.

2.3. Simulating horizontal fracturing in a limestone specimen

Another structure, simulating a system of fractures of horizontal, vertical or oblique orientation with the angles in a given range, can also be formed from ellipses. A system of elliptical fractures with a predominantly horizontal arrangement in a two-dimensional formulation of the problem is considered below.

The structure contained a network of elliptical fractures, arranged as 15 horizontal and 10 vertical rows with an incline of ±40° relative to the horizontal axis; the semi-major axis was 6×10^{-4} to 10.4×10^{-3} mm and the semi-minor axis was 1.2×10^{-4} to 2.8×10^{-4} mm. The deviations of the fracture centres from the uniform grid were ±4.9 mm horizontally and $\pm 8 \times 10^{-2}$ mm vertically. The fractures were located in a rock specimen 32×32×64 mm in size. When generating the size, incline and position of the ellipse centres, a random number generator with uniform distribution was used.

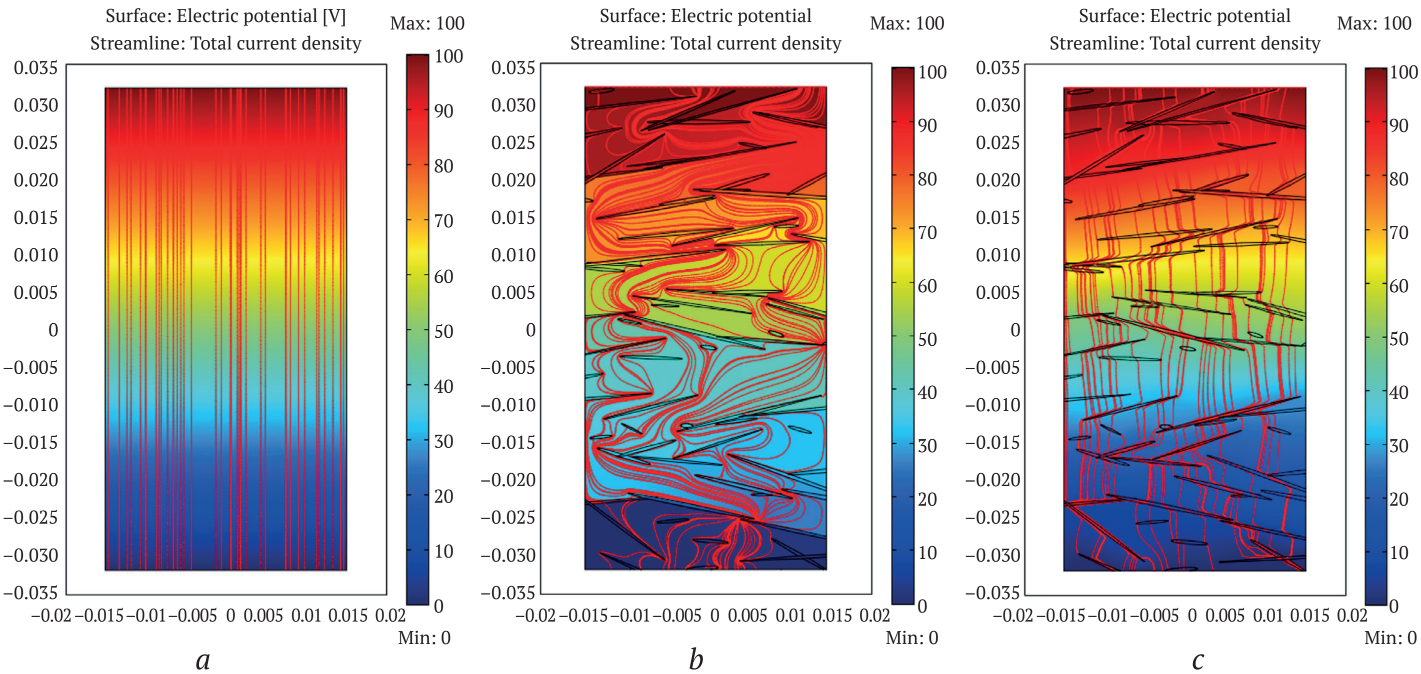
For the specimen of Cretaceous sediments, the rock conductivity was taken to be equal to the conductivity of limestone $\sigma_r = 10^{-4}$ Sm/m; the conductivity of water $\sigma_w = 10$ Sm/m; and the oil conductivity was taken to be 1×10^{-9} Sm/m. The values of conductivity of the media and the specimens are given in Table 2.

On the upper side of the specimen, a voltage of 100 V was set, relative to the lower side; the boundary condition of the lower side corresponded to ground. The simulation allowed us to obtain the distributions of the local current on the upper side of the specimen. In addition, in the course of the simulation, the lines of the electric current density were plotted, and the effective (averaged) specific electrical conductivity (EC) of the specimen was determined.

In the simulation, three cases were considered:

1) a homogeneous isotropic specimen without fractures;

2) a specimen with fractures filled with oil or air with low conductivity, less than the cement matrix conductivity;



a *b* *c*

Fig. 3. Current flow lines for specimens: homogeneous isotropic (*a*); with fractures filled with oil or air (*b*); with fractures filled with conducting saline water (*c*)

3) a specimen with fractures filled with saline water with high conductivity, greater than the matrix conductivity.

The calculated results are shown in Fig. 3 and Table 2.

The initial and simulated conductivities of the media and specimens are presented in Table 2.

Table 2

The conductivities of the media included in the model, as well as the averaged conductivities of the specimens: homogeneous isotropic; with fractures filled with oil or air; with fractures filled with conducting saline water

Medium	Homogeneous specimen	Fractures, oil	Fractures, saline water
Limestone	1×10^4		
Fracture filling	–	1×10^{-9}	1×10^1
Specimen	1×10^{-4}	4.304×10^{-6}	1.376×10^{-4}

For the homogeneous isotropic limestone specimen in Fig. 3*a*, the current flow lines are linear and directed vertically. Following on from the data in Table 2, for this specimen, exactly the same value of electrical conductivity was obtained for the rock, which was taken when forming the model.

For the specimen with fractures filled with low-conductivity liquid or air (in Fig. 3*b*), the current flow lines are bent, increasing the current path and decreasing the cross-section, that leads to decreasing the specimen's effective conductivity by more than 10 times.

For the specimen with fractures filled with conducting saline water, the conductivity increases by almost 40% due to the partial flow of current through the liquid.

Conclusions

1. The approach to the numerical simulation of heterogeneous structures containing elliptical inclusions generated from the Matlab programme, in conjunction with COMSOL Multiphysics (where finite-element simulation is performed), is quite effective.

2. The possibilities of simulating sandstones containing high-modulus grain-inclusions placed in a cement matrix have been demonstrated. The solution of the problem of determining local stresses in a specimen with such a structure under uniaxial strain in the direction of the longest side was considered. It was shown that the local stresses significantly exceeded the values averaged over the specimen's cross-sectional width; elongated areas of increased stress were present, oriented along the straining direction.

3. As an example of a fractured structure analysis, the influence of the filler on the electrical resistance of a limestone specimen, containing a system of thin, elliptical, predominantly horizontal fractures was considered. The change in the lines of current flow at different ratios between the matrix and the fracture filler conductivities and their effect on the effective (averaged) conductivity of the rock specimen was clearly demonstrated. The lower conductivity of the fracture filler leads to increased length and decreased cross-section of the current flow lines that, in turn, leads to a significant decrease of the conductivity of the fractured rock specimen. The higher filler conductivity results in slightly increased conductivity of the fractured specimen compared to that of the homogeneous isotropic specimen.

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