Numerical Study of Influence of Adsorbed Gas Filtration and Diffusion on Dynamic Phenomena in a Coal Seam

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Abstract. The connected physical-mechanical model of gas-saturated coal seam with explicit taking into the account the processes of filtration and diffusion of the gas mixture in the pores of the solid skeleton has been proposed. The developed model as been verified on the basis of experimental data on desorption of CO_2 from the sample of brown coal (lignite). An anomalous increase in strength and deformation capacity of gas-saturated coal sample during uniaxial loading in a certain range of pressure of gas in pores has been revealed. It has been shown that in this pressure range the destruction of the samples occurs with the formation of a large number of small fragments that can serve as a model of gas-dust emission into mine area.

1. Introduction

The presence of adsorbed gas in the coal seam produces a significant influence on the mechanical behavior of rock [1]. At the present time, the adsorbed gas in pores of a coal is often considered as the reason of instantaneous outbursts of large quantities of crushed coal, which constitutes a danger to human life and complicates the technological process.

There are two main types of pores in a coal: open pores and closed pores. Open pores are connected to the external surface and are directly accessible for gases and fluids. Open pores are further divided into “dead-end” or “interconnected” pores. Closed pores are completely isolated from the external surface and do not allow the access of external gases or fluids. Gas is retained in coal beds in four notable manners: 1) adsorption upon internal surfaces (in micropores); 2) absorption into the molecular structure of coal; 3) as free gas in voids, cleats, and fractures; and 4) as a solute in groundwater present within the coal seam. The question about physical state of gas, contained in coal, has been studied by many authors [2-4]. Although some details have not yet determined, it is regarded that methane is partially contained in the gas phase in the cracks, pores and macroscopic voids, and partially in adsorbed form as a film on the internal surfaces of pores and in the bulk of coal blocks [1].

Gas adsorption on the internal surface area of the coal is considered as most important mechanism for gas retention. The retention potential of coal is dependent on a number of factors including coal characteristics (rank, petrographic composition and mineral matter content) and physical parameters of the media (moisture, temperature, pressure, and gas composition, the last three influencing the gas compressibility factor).

The modern methods of computer-aided simulation allow the adequate description of the mechanical behavior of media in different states of aggregation. For example, to describe the mechanical behavior of solid medium there is a wide range of methods (finite difference, boundary element, cellular automata [5], et al), of which the most popular is the finite element method, as well as various types of particle method (discrete element, movable cellular automata [6] and other). Successful application of the movable cellular automata (MCA) method on the field of mechanical investigation of the lignite failure [7], dictated the further development with the incorporation of the conventional cellular automata (CCA) method. This development originated symbiotic cellular automata (SCA) method that enabled the possibility of investigation of the influence of mine gases. Mentioned approach was a result of long-term scientific collaboration between the Institute of Strength Physics and Materials Science SB RAS (Tomsk, Russia), the Velenje lignite mine (Slovenia), and the Faculty for the Natural Sciences and Engineering from University of Ljubljana (Slovenia).

Early the SCA method was verified within the simulation of sorption processes in lignite. The main aim of the present paper is to continue the development and improvement of the suggested approach in order to describe the multiphase system on example of Velenje lignite and to study the behavior of coal specimen in a gas atmosphere under external loading.

In the framework of the developed model the following assumptions have been made.

1. There is the coal, which represents the medium with open and closed porosity.
2. There is the mixture of ideal gases, which can pass in and out the coal sample.
3. Gases cannot be liquefied inside the pores of material. Under high pressures gases form immovable multi-layer film on the inner surfaces of pores.
4. The seepage of gas in the system of open pores and channels is described with Leibenzon equation for ideal gas [8].
5. The diffusion of gas between open and closed pores obeys to Fick law.
6. The temperature of whole system is considered as constant, due to high thermal capacity of solid framework, which is much bigger than thermal capacity of gas.

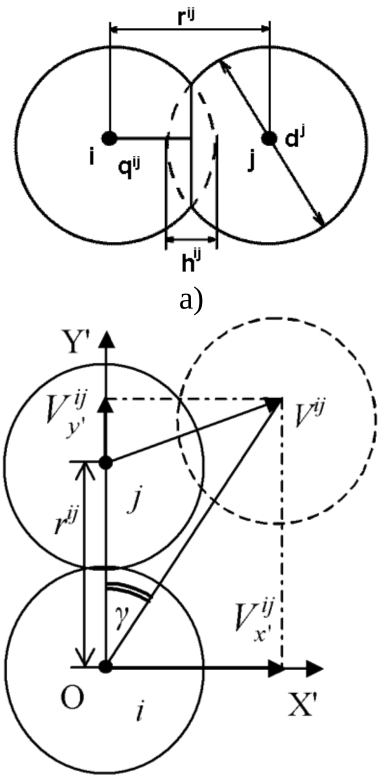
So, in this model there are two considered «types» of gas: 1) gas in open pores and channels, which can be treated as «fast» due to small characteristic time of filtration; and 2) gas in closed pores, and also dissolved gas, which can be considered as «slow», because of very long times of diffusion. Initially, this assumption, which proposes the existence of two characteristic times of sorption processes, was formulated in [9, 10].

2. Description of the method and main equations

In the framework of SCA method the step of calculation consists of two main substeps. First of them is the step of the MCA model, called «mechanical step». At this substep motion equations of movable automata are solved. In other words, the process of mass transfer and fracture of solid under mechanical loading is considered at the first substep. In the framework of the MCA method, we consider the simulated media as an ensemble of interacting finite size elements (automata) [6].

The concept of the MCA method is based upon conventional concept of cellular automata developed by means of incorporating of some basic postulates and relations of approach of particle-based methods [6]. The movable cellular automaton is an object of finite size, possessing translational and rotational degrees of freedom. Interaction between automata is defined by normal (acting along the line connecting the mass centers) and tangential forces, each of which is the sum of the corresponding potential and the dissipative components. Within the MCA approach a many-body interaction is used. Furthermore, new types of states, viz. the state of a pair of automata in comparison to conventional cellular automaton method are introduced. The new type of state leads to a new parameter which defines the criteria for switching of the inter-automata relationships – the automata overlapping parameter: $h^{ij} = r^{ij} - r_o^{ij}$ (Fig. 1a). Here r^{ij} is the initial distance between the centers of the neighboring elements, and r_o^{ij} is defined as $r_o^{ij} = (d^i + d^j)/2$, where $d^{i(j)}$ is the automaton size. In the simplest case there are two states of the pair: linked ($h^{ij} < h^{ij}_{max}$) and unlinked ($h^{ij} > h^{ij}_{max}$). h^{ij}_{max} means some critical value defined by investigated problem. The linked state is indicative of chemical bonds between elements and the unlinked state indicates that there is no chemical bond between them. According to the bistable automata concept (linked – unlinked) the Wiener-Rosenbluth model [11] can be used to define the normal potential force of interaction between *i*-th and *j*-th automata in approximation of nearest neighbors:

$$F_{np}^{ij} = p_{ij} + m_{ij}\left[\sum_{k\neq j} C(ij,ik)\left(\frac{1}{m_i}+\frac{1}{m_k}\right)p_{ik} + \sum_{l\neq i} C(ij,jl)\left(\frac{1}{m_j}+\frac{1}{m_l}\right)p_{jl}\right] \qquad (1)$$



a)

b)

Fig. 1: Definition of automata overlapping parameter (a) and shear stresses (b) in local coordinate system

Here $p_{ij(ik,jl)}$ is the corresponding pair potential force defined by the automaton response function; $m_{i(j,k,l)}$ is the mass of automaton and $m_{ij} = (m_i m_j / (m_i + m_j))$. The coefficients $C(ij,ik)$ are associated with the rate of perturbation transfer from pair ik to pair ij and were equal to unity. In the present realization of the MCA model a pair approximation is used to determine the tangential potential force $F_{\tau p}^{ij}$. Forces of inter-automata interaction consist of potential and viscous parts, where dissipative forces depend on relative normal and tangential velocities. In this case the relative overlapping can be considered as deformation in normal direction (ε^{ij}) and specific force (stress) σ^{ij} can be introduced for each automaton as normal force per contact square. In a similar manner it is possible to define shear strain γ^{ij} and stress τ^{ij} of i and j automata in i-j pair (Fig. 1b).

In the simplest case the linear approximation of real complex stress-strain curve can be used to represent the automaton response function in terms of stress (σ) and strain (ε). Depending on the simulated material properties the inter-automata interaction can be represented by response functions of different types. For example, the elastic properties of brittle materials can be described as simple linear response. In this case the loading and unloading will follow the same curve. To take into account the damage generation at a scale level lower than automaton size, the degradation response function should be used. In this case linear response is observed in the range of loading $<0\text{–}\sigma_{y1}>$, whereas in the range of $<\sigma_{y1}\text{–}\sigma_s>$ damage is generated within automata and the response function has non-linear character. In present model von Mises criterion was used as a criterion of strength and plasticity of the material. Previously, the MCA method was successfully used for the investigation of features of deformation, damages accumulation and fracture of various heterogeneous materials like concrete, porous ceramics, composite materials, interface materials like geological media [6, 12] and other.

Next for the mechanical – «net» substep is performed on the CCA mesh. At this substep the process of mass transfer of gas in the pores and channels is considered, as well as the values of the forces acting on the movable cellular automata from gas phase are calculated [12]. The configuration of pores and channels through which gas propagates, is projected to the CCA mesh from the MCA layer. Implemented model of gas filtration and diffusion is based on the following equations: 1) filtration equation for ideal gas:

$$\gamma \frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x}\left(\frac{k}{\mu} P \frac{\partial P}{\partial x}\right), \tag{2}$$

where γ – «open» porosity, ρ – density of gas; k – permeability of the coal; μ – viscosity of gas; P – partial pressure of gas; and 2) diffusion equation:

$$\gamma_0 \frac{\partial \rho}{\partial t} = \frac{3}{R} D \sqrt{\frac{1}{\pi(1-\gamma-\gamma_0/\nu)}} \frac{\partial^2 \rho}{\partial x^2}, \tag{3}$$

where γ_0 – «closed» porosity, R – mean radius of monolithic block of coal, D – diffusion coefficient, ν – solubility factor.

Initial concentration of dissolved gas in the material obeys to Henry's law:

$$\gamma_0 \rho = \nu P, \ \nu << 1. \tag{4}$$

The state of ideal gas in the model is described by Mendeleev-Klapeyron equation:

$$PV = NR_{gas}T,\qquad (5)$$

where N – number of moles of gas in considered volume V; R_{gas} – universal gas constant, T – temperature of gas. Permeability of the coal is estimated by following equation [10]:

$$k = \gamma d^2,\qquad (6)$$

where d – mean diameter of filtration channel, m.

Equations (2) and (3) are solved on the net of classical cellular automata by means of implicit numerical scheme. As we consider gases in the system as ideal, as we can calculate partial pressure of each gas independently. The calculation of sorption processes consists of two stages: 1) calculation of gas filtration (or seepage); 2) calculation of diffusion.

In order to describe the process of gas filtration, the equation (2) should be supplemented with initial and boundary conditions. At each step of simulation, the distribution of gas pressure in open pores and in outer space is considered as initial conditions for current step. The setting up of boundary conditions is more complex problem. It is evident, that simulated object can consists of three types of classical cellular automata: 1) CCA, belonging to macropores or outer space of specimen; 2) CCA, belonging to coal, with open pores and channels and with closed micropores; and 3) CCA, belonging to some impermeable material, which cannot pass gas(es), like steel walls of vessel and so on. Thus, there are two types of boundary conditions: 1) «macropore ↔ coal»; and 2) «impermeable material ↔ coal».

Calculation of influence of pressure of gas, containing in voids and crystal lattice of porous solid, on solid-phase framework can be done using different methods (one of them is reported in [13]). At present time simpler model is realized. Within the framework of this model pressure influence of gas contained in filtration volume and closed pores is considered as proportional to porosity value. So, pressure on the solid-phase framework of cellular automaton is calculated as follows:

$$P_{gas} = P_{closed}\gamma_0 + P_{open}\gamma,\qquad (7)$$

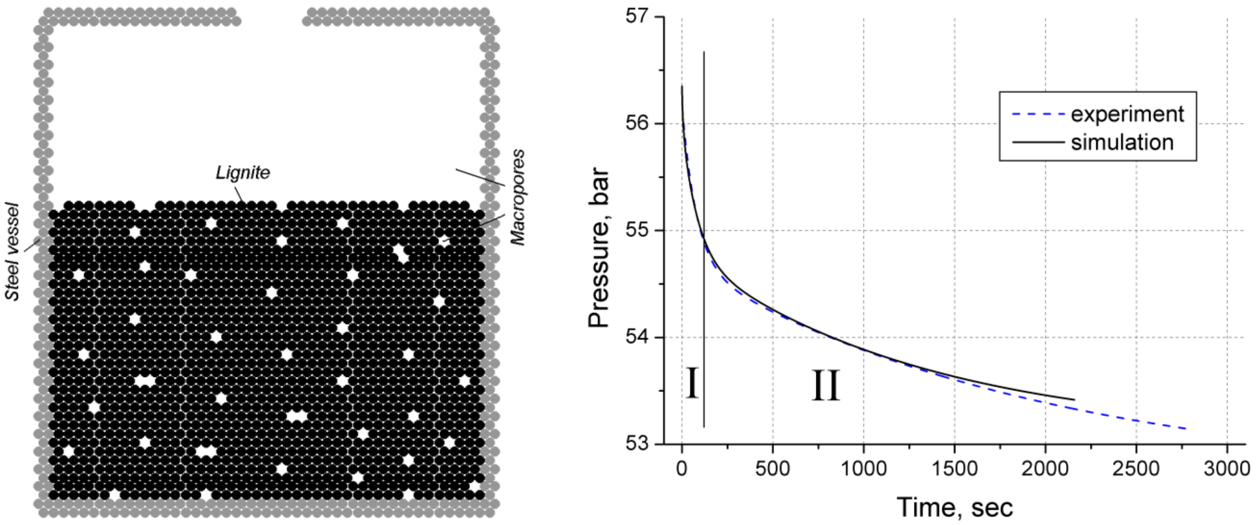
where P_{open} and P_{closed} are total pressures of gas in filtration volume and closed pores of automaton. Gas-induced internal pressure P_{gas} on solid-phase framework is added to mean stress in movable cellular automaton. Expression (7) implies uniform distribution of pores, cracks and channels in the volume of cellular automaton. It also means that diameter of automaton is several orders of magnitude higher than mean size of monolithic blocks in simulated porous solid. Note that within the framework of present model influence of absorbed gas molecules (molecules located in crystal lattice) on increase of elastic energy of solid-phase framework is not taken into account.

3. Verification of the model of gas filtration and diffusion

The developed model of contrast porous medium was verified by means of comparison with results of experimental tests, made by J. Zula and Prof. J. Pezdic [14] from Faculty of natural sciences and engineering, University of Ljubljana, Slovenia. Methods of tests and experimental equipment are described in detail in [15]

The parameters of model specimen were set up the same as in the experiment (Fig. 2a). Volume of the vessel was 105 ml, mass of fine detritus in the vessel was 60 g. The pressure of CO_2 in vessel was increased sharply (practically instantly) from atmospheric pressure to 56.3 bar. After that the decrease of pressure in the vessel was observed. Qualitatively good compliance between experimental data and simulation results was obtained (Fig. 2b). The resulting estimates of parameters of lignite are given in Table 1.

The dependence, shown in fig. 2b, consists of two parts: 1) relatively fast decrease of pressure due to filtration of CO_2 into open pores and 2) slow decrease part, during which the diffusion of gas into closed porosity plays the main role. Obtained behavior of model is in compliance with theoretical assumptions about the physical nature of processes, which take place during sorption of gas. This confirms the correct formulation of the problem and qualitatively correct description of the basic processes occurring in the system.



a) b)

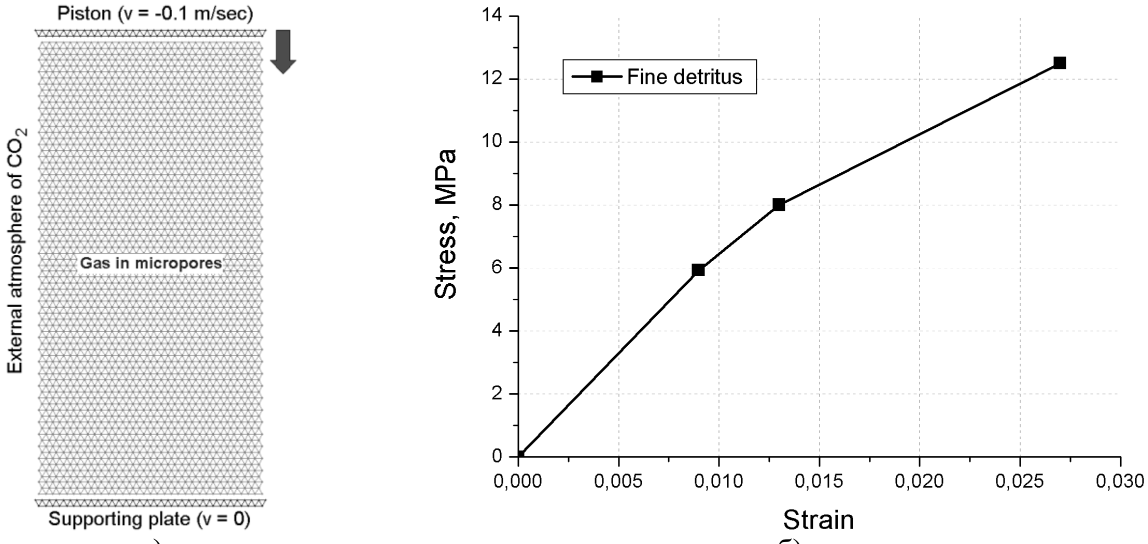
Fig. 2. Scheme of simulated specimen (a), the dependence of pressure in the vessel on time (b)..

Table 1. Estimates of parameters of lignite (on the basis of J. Zula experiments).

Open porosity	0.02	Diffusion coefficient, cm^2/sec	$2 \cdot 10^{-7}$
Closed porosity	0.4	Solubility factor	0.05
Mean diameter of filtration channel, m	$2.5 \cdot 10^{-9}$	Mean size of «monolithic» block, m	$1 \cdot 10^{-4}$

4. Simulation of mechanical response of gas-filled coal specimens

The study of the mechanical response of gas-filled lignite specimens to uni-axial loading with constant velocity $v = 0.1\ m/\sec$ has been carried out (Fig. 3a). Pressure of external atmosphere was 1 bar. The specimen was fixed between steel matrix and piston. Mechanical properties of pair of movable cellular automata corresponded to mechanical properties of fine detritus, which is one of the lithotypes of lignite (Fig. 3b). Structure of lignite specimen was uniform, macroscopic pores and inclusions were absent.



а) б)

Fig. 3. Scheme of simulated specimen (a), mechanical properties of simulated material (fine detritus) (b).

According to obtained results, specimens show brittle type of fracture, which is carried out by means of formation of one or several diagonal cracks, extending from corners of the sample.

Revealed an anomalous character of the dependence of strength of the samples on the gas pressure in the pores (Fig. 4). Thus, in the pressure range from 32 to 48 bar the increase of the strength of samples by 15-20% is observed, while the total dependence of the strength of the gas pressure tends to decrease. The detailed investigation of the destruction of samples at different gas pressures in the pores showed that in the pressure range from 32 to 48 bar the localization of deformation near the matrix and the punch is not expressed. On the contrary, the deformation is distributed fairly evenly over the specimen. This fact is confirmed by histograms of the distribution of intensity of deformations (Fig. 5a).

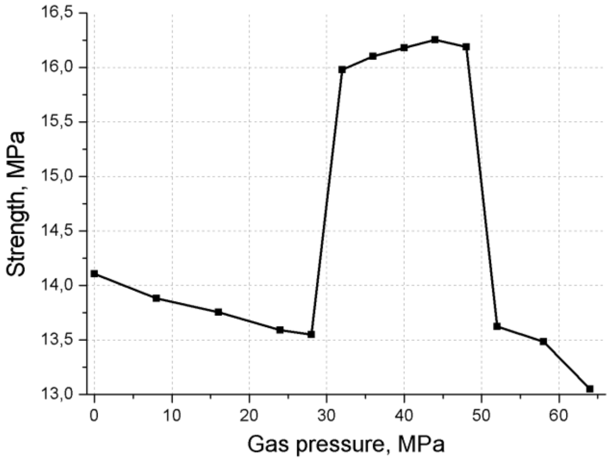
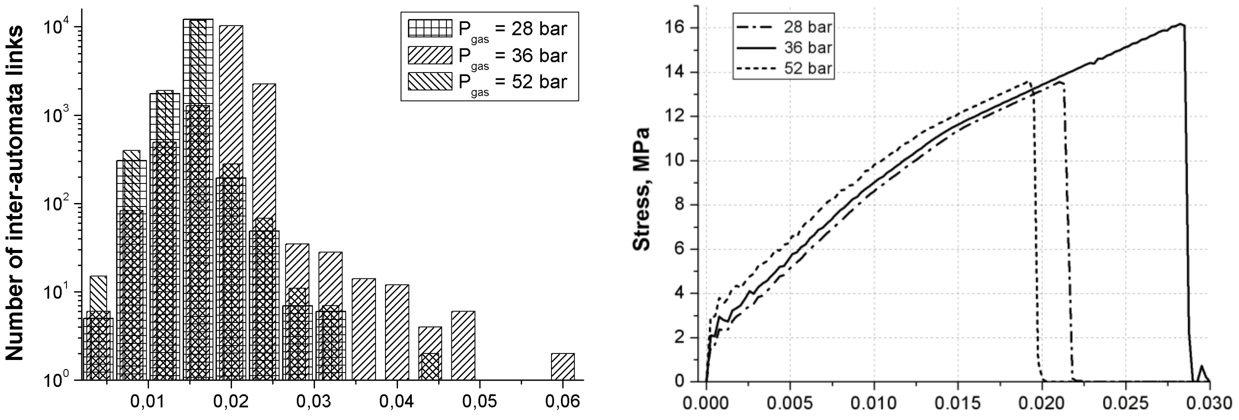


Fig. 4. The dependence of strength of gas-filled specimens on the pressure of gas in the pores.

As can be seen from Fig. 5a, at a pressure $P_{gas} = 36\,bar$ at the final stages of loading, immediately preceding the fragmentation of the sample, the proportion of inter-automata links, subjected to relatively large strains, becomes significantly higher than that for specimens under pressures $P_{gas} = 28\,bar$ and $P_{gas} = 52\,bar$. Thus, the internal gas pressure in a certain range of values leads to a «plasticization» of the material and increase its deformation capacity. As a result, the deformation capacity, and thus the mechanical strength of the samples increase (Fig. 5b).

Depending on the gas pressure in the pores, the character of damage accumulation in the specimen during the loading may be different. For example, at pressures from 32 to 48 bar sufficiently large damaged areas formed at the corners of the specimen, however, extended cracks are absent. At $P_{gas} < 32\,bar$ and $P_{gas} > 48\,bar$ during the compression of the specimen cracks begin to form in the corners of specimen. These cracks are oriented at an angle of 60 degrees to the vertical; the formation of small disconnected damages is practically not observed.



а) б)

Fig. 5. Histograms of distributions of strain intensity in the inter-automata links at the final stage of loading of the samples (a) and diagrams of the loading of samples (b) at different gas pressures in the pores.

The character of the fragmentation of the specimens at different pressures in general remains brittle, but varies in detail with variation of the gas pressure in the pores (Fig. 6). For gas pressures less than 32 bar and higher than 48 bars, the samples are destroyed by the formation of the two main cracks from the upper or lower corners with a small amount of fragments. For pressures in the range from 32 to 48 bars pattern of destruction is somewhat different. In this case main crack crosses the specimen from left to right and top to bottom, with the formation of many small fragments in the middle of the specimen. Such behavior can simulate the formation of dust-gas outburst from coal seam, in which crushed coal particles, mixed with desorbed gases, are ejected into space of mine.

а) $P_{gas} = 28\,bar$ б) $P_{gas} = 36\,bar$ в) $P_{gas} = 52\,bar$

Fig. 6. Fragmentation of specimens under different pressures of gas in the pores.

5. Summary

The approach, describing the behavior of two-phase medium under external influence, is proposed. This approach, called as SCA method, represents the combination of methods of conventional and movable cellular automata.

The obtained results of simulation of uniaxial compression of gas-saturated coal specimens show that the gas pressure in the pores of the material produces a significant effect on its mechanical properties. Note that values of pressure of gas were below the limit of elasticity, respectively, in the absence of an external loading gas-saturated specimens did not experience significant strain and, moreover, not destroyed.

Influence of gas pressure in the pores on the mechanical properties and fracture of specimens has nonlinear character. The increase of strength and deformation capacity of the material is accompanied by a change in the mode of its fracture, in particular, the geometry of the main crack and a significant increase of the number of fragments.

The most important result of the research is the revelation of the loading parameters, in which there is considerable fragmentation and «explosive» behavior of fracture of the sample, with previous increase of the mechanical strength and deformation capacity during the loading. This result can be used for prediction of hazardous areas in a coal seam.

In the framework of these studies, the coal specimen was assumed to be homogeneous, while real materials are expressed by a heterogeneous structure. The study of the influence of the structure of the specimens on their mechanical response is one of the problems to be solved in the future.

The method of symbiotic cellular automata, used in the paper, is universal and can be applied to describe the behavior of a wide class of contrast media consisting of components in solid, liquid and gaseous phases.

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