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SIMULATION OF THE MECHANICAL RESPONSE OF FLUID-SATURATED POROUS MEDIUM WITH HYBRID CELLULAR AUTOMATON METHOD

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Abstract. The connected physical-mechanical model of fluid-saturated porous medium, based on the coupling of particle method and net method, has been proposed. The model has been applied to simulation of the mechanical response of gas-saturated brittle material under uni-axial loading. An anomalous increase in strength and deformation capacity of samples 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

Many technical and natural objects and materials represent fluid-saturated porous media. Striking examples of such media are porous geological seams filled with a mixture of liquids and gases, biological materials (bone tissue filled with liquid), etc. Study of a mechanical response of these media under mechanical loading represents one of the actual problems being on a joint of materials science, the theory of elasticity and plasticity, dynamics of liquids and gases. At that, as analytical as numerical researches by means of traditional and widely known methods of simulation are complicated due to the absence of the advanced approaches allowing adequate description of interaction of components of media, being in various aggregate states at different scales. In order to solve the abovementioned problem, the hybrid cellular automaton (HCA) method has been developed. The main idea of this method is to join together particle method and net method [1-3].

In order to correctly describe a porous medium, it is necessary to accurately take into the account the porosity of material. In the framework of proposed model we assume that there are two main types of pores in a porous material: open pores and closed pores. Open pores are connected to the external surface and are directly accessible for gases and fluids. Closed pores are completely isolated from the external surface and do not allow a filtration of gases or fluids. Speaking about the gaseous fluid, it is necessary to note, that gas can retain in porous material in four notable manners: 1) adsorption upon internal surfaces (in microscopic pores); 2) absorption into the molecular structure of material; 3) as free gas in voids, cleats, and fractures; and 4) as a solute in liquid(s) present within the material.

The main aim of the present paper is to study the effect of gas phase on the mechanical response of gas-saturated porous medium under uni-axial loading. In the framework of the developed model the following assumptions have been made.

1. The material under consideration represents the medium with open and closed porosity.
2. There is the mixture of ideal gases, which can pass in and out the 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.
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 higher 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 [4].

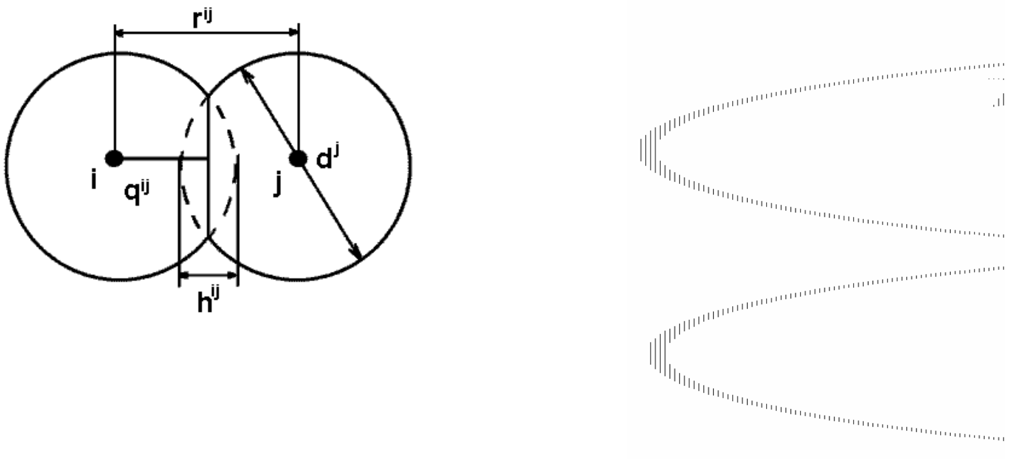
2 DESCRIPTION OF THE METHOD AND MAIN EQUATIONS

In the framework of HCA method the step of calculation consists of two main substeps. First of them is the step of the movable cellular automaton (MCA) model, called «mechanical step». At this substep motion equations of movable automata are solved, in other words, the processes of mass transfer and fracture of solid under mechanical loading are considered. In the framework of the MCA method, we consider the simulated media as an ensemble of interacting finite size elements (automata) [5,6].

The concept of the MCA method is based upon the conventional concept of cellular automaton developed by means of incorporating of some basic postulates and relations of approach of particle-based methods [5,6]. 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 the 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 a 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 [7] can be used to define the normal potential force of interaction between *i*-th and *j*-th automata in approximation of nearest neighbors:

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

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).



a) b)

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

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 $<0–\sigma_{y1}>$, whereas in the range of $<\sigma_{y1}–\sigma_s>$ damage is generated within automata and the response function has non-linear character. In the 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 [5,6] and other.

Next for the mechanical – «net» substep is performed on the classic cellular automaton (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 [2]. 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 a gas; k – permeability of the porous material; μ – viscosity of gas; P – partial pressure of gas; and 2) diffusion equation:

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

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

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

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

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

$$PV = NR_{gas}T, \tag{5}$$

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

$$k = \gamma d^2, \tag{6}$$

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 automaton: 1) CCA, belonging to macroscopic pores or outer space of specimen; 2) CCA, belonging to material 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 ↔ porous material»; and 2) «impermeable material ↔ porous material ».

Calculation of influence of pressure of gas, containing in voids and crystal lattice of porous solid, on solid-phase framework can be performed by various methods (one of them is reported in [8]). At present time the simpler model is implemented. In the framework of this model the pressure influence of gas contained in open and closed pores is considered as proportional to porosity value. So, the pressure on the solid-phase framework of cellular automaton is calculated as follows:

$$P_{gas} = P_{closed}\gamma_0 + P_{open}\gamma \ , \tag{7}$$

where P_{open} and P_{closed} are total pressures of gas in open 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 much 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. The parameters of porosity, which were used in following calculations, are shown in Table 1. These estimates are based upon the experimental data on sorption properties of porous brown coal (lignite) from [10].

Table 1. Estimates of parameters of porous material

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	$1{\cdot}10^{-4}$

3 SIMULATION OF MECHANICAL RESPONSE OF GAS-SATURATED SPECIMENS

The study of the mechanical response of gas-filled specimens to uni-axial loading with constant velocity $v = 0.1\ m/\sec$ has been carried out (Fig. 2a). 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 brown coal (lignite) [10]. (Fig. 2b). Structure of specimens was uniform, macroscopic pores and inclusions were absent.

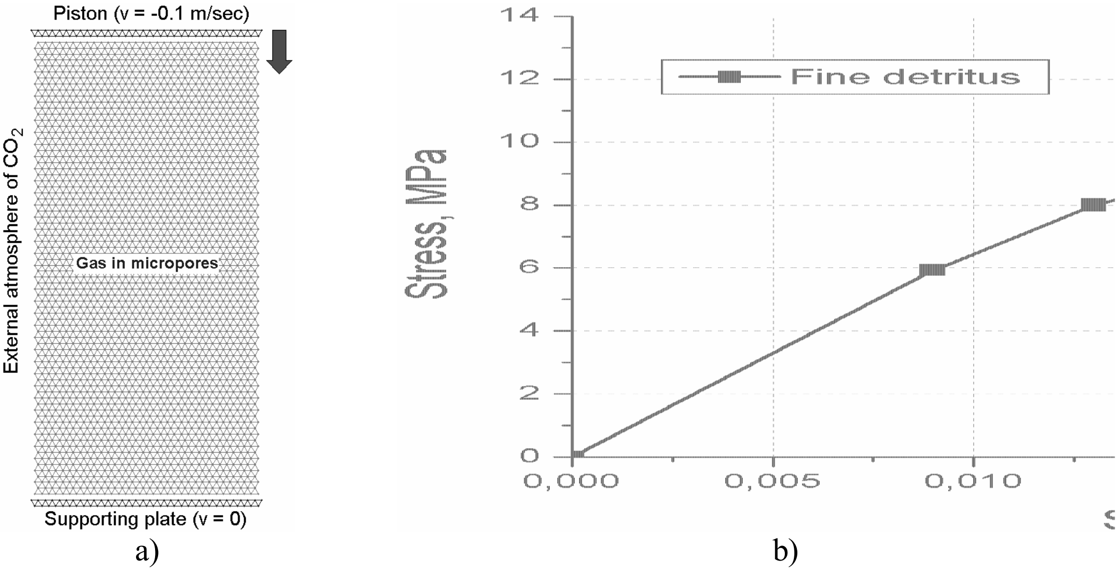


Figure 2: Scheme of simulated specimen (a), mechanical properties of simulated material (b).

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. 3). 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. 4a).

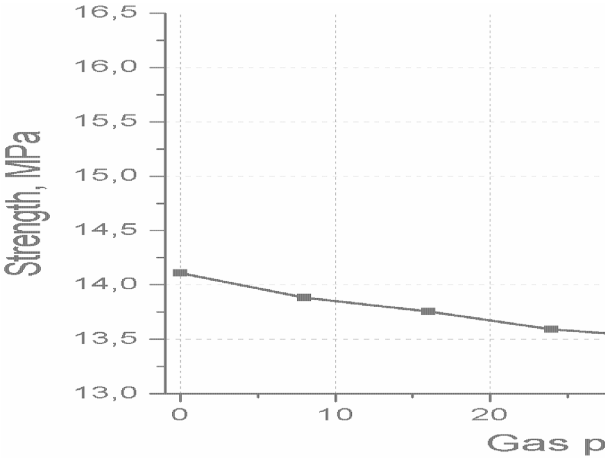
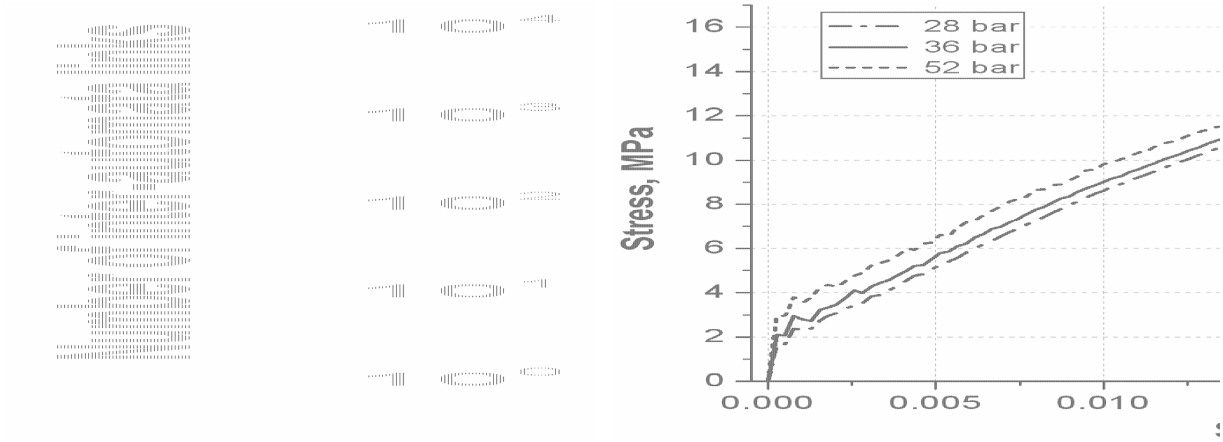


Figure 3: The dependence of strength of gas-saturated specimens on the pressure of gas in pores.

As can be seen from Fig. 4a, at the 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 increases its deformation capacity. As a result, the deformation capacity, and thus the mechanical strength of the samples increase (Fig. 4b).

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.



a) b)

Figure 4: 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. 5). 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.

a) $P_{gas} = 28\ bar$ b) $P_{gas} = 36\ bar$ c) $P_{gas} = 52\ bar$

Fig. 5. Fragmentation of specimens under different pressures of gas in the pores.

4 CONCLUSIONS

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

The obtained results of simulation of uni-axial compression of gas-saturated specimens show that the gas pressure in the pores of the material has the 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. The observed 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 the 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 further development of methods of prediction of hazardous areas in a coal seam.

In the framework of these studies, the specimen was assumed to be homogeneous, while many natural 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 hybrid cellular automata, described in the paper, is universal and can be applied to study the behavior of a wide class of contrast media consisting of components in solid, liquid and gaseous phases.

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