APPLICATION OF HYBRID CELLULAR AUTOMATON APPROACH FOR COMPUTER-AIDED EXAMINATION AND FORECAST OF STRENGTH PROPERTIES OF HETEROGENEOUS COAL-BEDS

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ABSTRACT

One of the modern and perspective applications of computational mechanics is investigation of complex multiphase media containing components in different aggregative states. Striking examples of multiphase media are coal-beds, soils, geological medium and so on. In the present paper the new method for simulation of response and fracture of multiphase media, the hybrid cellular automaton method, is proposed. Developed approach was applied for computer-aided simulation of response and fracture of lignite under complex boundary conditions imitating real-life environment in coal beds. Simulation results show that presence of constrained boundary conditions can lead to change of lignite fracture regime in the range from brittle to quasi-viscous. In the case of hard boundary conditions increase of surrounding material hardness leads to transition from brittle fracture of fined detritus to degradation regime, which is characterized by generation and accumulation of numerous damages. As a result at slump of lateral pressure (in practice this situation is realized during mining or digging) fine detritus can demonstrate explosion-like fracture. In the case of boundary conditions realized by means of applied force (this type of boundary conditions is the most close to real conditions in coal beds) the vice versa dependency for fined detritus is observed. Here explosion-like regime is observed at lateral pressure slump in the case of soft surrounding material. Proposed hybrid cellular automata concept can be efficiently used for solving various geo-mechanical, biological, engineering and materials science tasks, which consider heterogeneous multiphase objects.

1 INTRODUCTION

The probability of foundering of roof and walls of coal mines is one of the central problems in the coal-mining industry (Brady [1]). Consequently, reliable knowledge about strength characteristics, conditions and type of lignite fracture is critically important to guarantee safety of coal mines as well as adjoining earth-based and underground objects. Inasmuch as now intensive mining is carried not only in Slovenia but all over the world, problems of safety directly concern of life and death of millions of people working in coal mining industry.

Lignite is very complex material for investigation due to its heterogeneity and considerable absorbing capacity (Markich [2], Kanduč [3]). Depending on lithotype structure the character of lignite response and fracture can vary from quasiplastic to brittle. Presence of a big quantity of absorbed gases presents additional complexity for understanding of lignite behavior. Quick desorption of gases during initiation of cracks and damages as well as during changing of stress-strain state of material potentially can lead to lignite fracture of explosion type.

The strength characteristics and the bearing capacity of lignite are traditionally investigated using a set of standard tests, viz., compression, tension, shear tests etc (ISRM, [4]). However, data obtained in such a way are not necessarily sufficient to predict the behavior of the test material under complex real conditions. This is primarily due to the fact that lignite seams occurring at great depths experience triaxial compression that is greatly different from the conditions near the surface and, particularly, near tunnels.

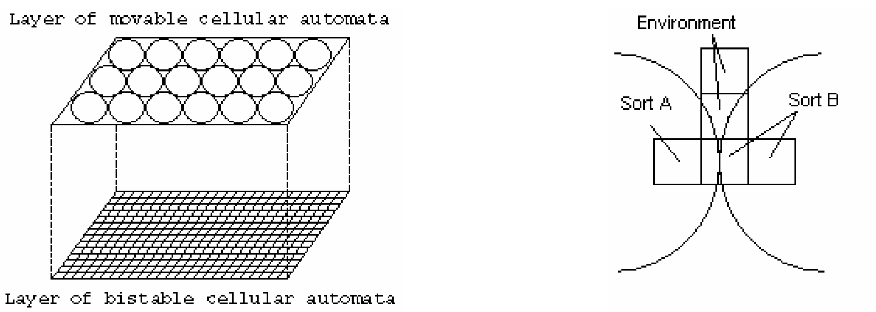
Described problems can be solved using computer-aided simulation that can reproduce original conditions of lignite bedding and predict its mechanical properties under real conditions of coal beds. And furthermore, it can predict processes in the coal beds after laying the tunnels or other mining activities. In the present paper the new and very promising Hybrid Cellular Automata method was applied for investigation of response and fracture of lignite under mechanical loading with taking into account gas sorption on the coal.

2 DESCRIPTION OF THE HYBRID CELLULAR AUTOMATON METHOD

One of the most perspective applications of computational mechanics is investigation of complex multiphase media. At the present time there are several approaches allowing simulation of such kind of tasks. They are based on conventional cellular automaton approach that makes possible modeling of processes of heat and mass transfer in complex heterogeneous medium under dynamic impacts. Two methods can be marked out: the movable cellular automaton (MCA) method allowing direct simulation of fracture processes under mechanical loading (Psakhie [5-7]) and conventional method of bistable cellular automata (BCA) that is usually used for description of heat transfer, chemical reactions, gas diffusion, fluid percolation and adsorption-desorption processes (Wolfram [8-9]).

The new approach combining advantages of both conventional BCA and MCA methods was developed. This method is called as a hybrid or symbiotic cellular automata method. In the framework of this method investigated medium is considered as a superposition of two interrelated media. The first one is described by the ensemble of movable cellular automata, and the second one is the net of conventional cellular automata (Fig.1,a).

In the framework of hybrid method the step of calculation consists of two main sub-steps. First of them is the step of the MCA model ("mechanical step"). Motion equations of movable automata and energy dissipation at the expense of internal friction and plastic deformation are calculated on this sub-step (Psakhie [5]). After that physico-mechanical properties of movable automata are "projected" on the net of conventional bistable cellular automata (Fig.1,b). On the second sub-step ("net step") the layer of bistable cellular automata is considered. Processes of heat transfer, liquid and gas dynamics, redistribution of gas pressure and so on are simulated. At the end of this step recalculated parameters of bistable automata are projected on the set of movable automata.



a) b)

Figure 1: a) two "layers" of the considered medium; b) projection of the "MCA layer" to the "BCA layer".

Note that the algorithm of projection of movable automata on unmovable net takes into account degree of overlapping of automata and unmovable cell. For example in the case of superposition of two automata on the cell the sort of the cell (xylite, fine detritus and so on) is defined by the sort of movable automaton that occupies the most part of the cell (Fig.1,b). The state of this cell is solid. The cell, which is not occupied by any movable automaton, has another state – gaseous or liquid state. This cell is a part of surroundings and can be filled by gas or fluid. In the case of gas state it is characterized by temperature T, pressure P and gas (or gases) molar concentration μ. This cell is not taking part in mechanical behavior of the system but influences on neighboring movable automata by gas pressure.

The simplified model of equidistribution of gas concentration in closed free volume ar each time moment was used in the carried out investigation. In the framework of this approximation every cell of closed free volume has the same value of temperature, molar concentration of gas (or gases) and pressure. After mechanical step finish the shape, volume and quantity of gases (CO_2 and CH_4) in each new closed region is recalculated. The temperature of the closed volume is recalculated by the same way as gas molar concentration (new average value is calculated). Gas acts on movable automata of free volume walls with an additional force, which is applied to mass centers of automata. Change of mean stress in the volume of movable automata due to gas pressure is also taken into account in the model.

Simulated porous specimen has boundaries between solid material and closed free volumes and surroundings filled by gases. There are two types of sorption processes on these boundaries: adsorption of gas on the surface of solid phase and desorption of gas to the volume of pore, crack or surroundings. In very wide range of gas concentrations it is possible to consider adsorption and desorption processes as independent. In the simplest case they are described by the following linear equations:

$$\begin{cases} I_{ads} = \alpha_{ads} C_{gas} \left(C_{gas}^{\max} - C_{gas}^{material} \right) \\ I_{des} = K_{des} \left(C_{gas}^{material} - C_{gas}^{\min} \right) \end{cases}.$$

Here I_{ads} and I_{des} are adsorption and desorption intensities correspondingly ([mole/(m^2*s)]); C_{gas} is the local value of molar concentration of gas near the surface of the sample ([mole/m^3]); $C_{gas}^{material}$ is the current local value of molar concentration of gas in material near the surface (in the boundary symbiotic cell) ([mole/m^3]); $C_{gas}^{\min}$ and $C_{gas}^{\max}$ are the minimum and maximum possible molar concentrations of gas in porous material ([mole/m^3]). In general case α_{ads} ([m^4/(mole*s)]) and K_{des} ([m/s]) are the functions of material and gas parameters. In carried out investigations α_{ads} and K_{des} were considered as constants.

Possibility of phase transformation from gaseous to liquid state at critical pressure was not taken into account in the present model.

3 DEFINITION OF SORPTION COEFFICIENTS

As was mentioned above, the lignite has organic nature and consists of solid skeleton and numerous micro-pores, fractures and microfractures. These discontinuities are filled by various gases (mostly by $C0_2$ and CH_4). In the present work influence of $C0_2$ and CH_4 on lignite response and fracture was taken into account.

Lignite has to main constituents: fine detritus and xylite. Lignite lithotype categories are defined on the base of xylite (or fine detritus) volume fraction. Note that lignite in the coal seam is under high pressure (up to 80 bars). So, determination of coefficients of sorption of $C0_2$ and CH_4

on two main lignite constituents under high pressures (from 30 to 80 bars) allows us to simulate lignite response during changing conditions in coal seams.

Sorption coefficients α_{ads} and K_{des} were calculated using experimental data from (Pezdič [10]) and are presented in the Table 1. Referenced experiments of sorption on lignite were carried out at high pressures (up to 100 bars) using special technique. The lignite specimens were cut into little pieces with diameter between 1 and 7 mm and put into reaction vessel. Volume content of lignite pieces in the vessel was about 50% for all specimens. After evacuation the chosen gas ($C0_2$ or CH_4) was compressed over coal. The gas introduction time into reaction vessel was 10 to 15 seconds. Then the value of gas pressure in the vessel was measured during several hours. Desorption properties of different lithotypes coal were defined using the similar procedure. After finishing adsorption measurements the gas was evacuated from the vessel during 10-15 seconds (the value of gas pressure at the end of this stage was about 1 bar). Then change of gas pressure in the vessel was measured during several hours (like in adsorption experiments).

Table 1. Coefficients of sorption of $C0_2$ and CH_4 on xylite and fine detritus (FD).

	CO_2 / xylite	CO_2 / FD	CH_4 / xylite	CH_4 / FD
α_{ads} , m^4/(mole*s)	$2.9*10^{-8}$	$4.0*10^{-8}$	$1.4*10^{-8}$	$1.3*10^{-8}$
K_{des} , m/s	$3.1*10^{-5}$	$2.6*10^{-5}$	$3.0*10^{-5}$	$2.7*10^{-5}$

To verify the developed model the computer-aided simulation was realized using hybrid cellular automata method and described above model of sorption. The conditions of the simulated system imitated the real conditions in the experiments. Comparison of the simulation results with experimental data shows that developed model describes correctly sorption process at the values of gas content in the material, which are close to upper ($C_{gas}^{\min}$) or lower ($C_{gas}^{\max}$) limit. In other words, the model works properly during first minute of simulated adsorption or desorption process. Note that typical time of simulated dynamic processes in the coal seam doesn't exceed 10 seconds. So, proposed simplified model of sorption is right for simulation of dynamic mechanical tasks, which concern, for example, response and fracture of constrained volume of coal during sudden change of physico-mechanical state of surrounding material.

4 INVESTIGATION RESULTS AND DISCUSSION

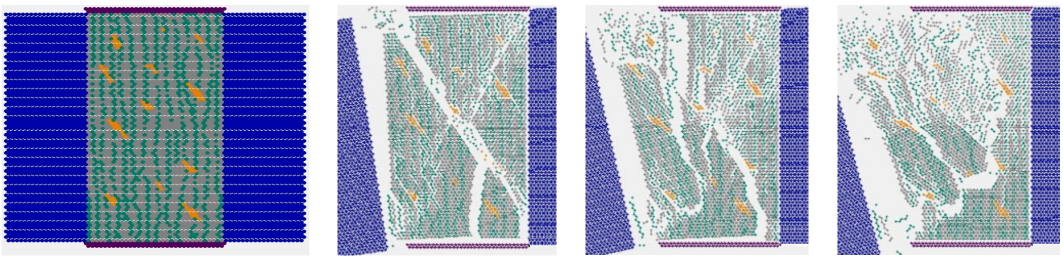
Developed hybrid cellular automaton approach was applied for computer-aided simulation of response and fracture of lignite under constrained boundary conditions imitating real-life environment in coal beds. Two lithotype categories of lignite were considered: fine detritus (lithotype code 10) and xylite (lithotype code 4). Mechanical response functions of xylite and fine detritus were fitted to experimental loading diagrams of degassed standard cylindrical specimens (diameter 5 cm, height 10 cm) under uniaxial compression (Psakhie [7]).

The typical set-up for carrying out the tests is shown in the Figure 2,a. Considered specimen of fine detritus of xylite is surrounded by upper and lower punches and two side "layers". The response function of side walls was linear-elastic with infinite strength. The value of Young modulus of surroundings E_s was varied from $0.3\times E_{fD}$ to $3\times E_{fD}$ (E_{fD} is Young modulus of tested lignite lithotype). Note that different values of E_s imitate different surrounding materials or different states (concentrations of damages and cracks) of surrounding material in the coal seam.

Two types of constrained boundary conditions were considered: applied deformation and applied force. The first one was realized by fixing the outer boundaries of side walls and bottom layer of automata of the supported plate (lower punch) and by applying constant velocity load to the upper punch. The second type of boundary conditions includes applying horizontal compression force to outer boundaries of side walls and vertical compression force to lower and upper punches. Different values of applied vertical deformation ε_v or pressure σ_v imitate stress-strain state of coal at different depths. In case of applied force the values of σ_v varied from 8MPa (corresponds to the depth 400m) to 16MPa. The value of horizontal (side) pressure σ_h was constant and equal to 6.4 MPa. In case of applied deformation the maximum value of ε_v was 2.75% that corresponds to different values of normal vertical stress depending on Young modulus of side layers.

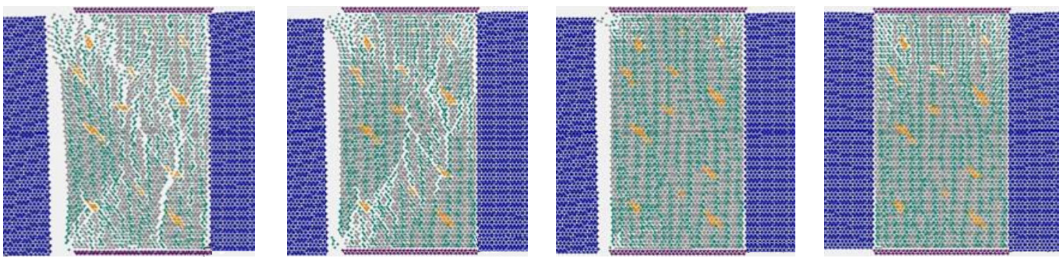
Mining or digging change (sometimes dynamically) stress-strain state of considered volume of coal. Note that dynamic action can lead to serious consequences for mines in the form of coal outbursts in the tunnels. To investigate dependence of coal fracture regime on state of surroundings the following procedure was used. After reaching given loading conditions and "relaxation" stage the both punches and the right wall were fixed and the left side wall was set free. Fracture of the coal specimen was analyzed.

Figure 2,b-d shows fracture of fine detritus specimen under "applied deformation" boundary conditions at three different values of Young modulus of side walls. Analysis of simulation results shows that typically brittle fracture of fine detritus is observed at "soft" side walls (E_s<E_{fD}). Note that such fracture regime is typical for detritus specimens with free sides (Fig.2,b). Number of damages and cracks as well as velocity of flying away of coal fragment increase with increase of E_s (Fig.2,c-d). It is seen that the specimen demonstrates explosion-like fracture in case of "hard" side walls (Fig.2,d). Underscore that σ_v decreased to 3-4MPa after this procedure in case of E_s=0.3×E_{fD} and E_s=E_{fD} while the specimen became totally destroyed (σ_v=0) in case of "hard" side walls.



a) b) c) d)

Figure 2: Initial structure of the set-up (a) and fracture patterns of the fine detritus specimen after left wall freeing (ε_v=2.75%): b) E_s=0.3×E_{fD}; c) E_s=E_{fD}; d) E_s=3×E_{fD}.



a) b) c) d)

Figure 3: Fracture patterns of the fine detritus specimen after left wall freeing (σ_v=16MPa): a) E_s=0.33×E_{fD}; b) E_s=E_{fD}; c) E_s=3×E_{fD}; d) E_s=E_{fD} (another procedure).

Figure 3,a-c shows fracture of fine detritus specimen under "applied force" boundary conditions at three different values of Young modulus of side walls (σ_v=16MPa). The inverse dependence of fracture regime on hardness of side walls is observed here. Fracture regime, which is closer to explosive type, is observed at small values of E_s (E_s<E_{fD}). The specimens constrained by "hard" side walls (E_s>E_{fD}) became undestroyed (some damages in the specimen presented in the Fig.3,c were accumulated during preliminary loading). The "residual" value of σ_v increases with increase of E_s. Underscore that fine detritus specimen kept some bearing capacity (non-zero value of σ_v) at all set values of E_s and "initial" σ_v.

Influence of left wall freeing rate on lignite fracture regime was also analyzed. Figure 3,d shows fracture pattern of the set-up with E_s=E_{fD} after relatively slow removal of the left wall (σ_h was linearly decreased from initial 6.4MPa to 0). Comparison of this figure with Fig. 3,b shows that parameters of dynamic "unloading" of the constrained specimen are not of less importance than hardness of surroundings. Note that similar results are observed for other in case of other E_s and σ_v.

Testing of constrained xylite specimens doesn't reveal explosive-like fracture at any values of E_s, σ_v and ε_v.

Note that "applied force" boundary conditions correspond to fault region in the coal seam, argillaceous formation roof or regions of coal with argillaceous admixture. Simulation results demonstrate the possibility of hazardous brittle fracture of detritus in case of sudden local changes of stress-strain state in the seam. Brittle fracture with elements of explosive fracture is observed in case of "applied deformation" boundary conditions. In spite of the fact that such type of boundary conditions is infrequent in coal seams, they are very dangerous for mine tunnels.

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