Cellular-automaton modeling of gas sorption kinetics in the finite volume of coal

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Abstract. The work is devoted to cellular-automaton modeling based on a class of cellular automata with Margolus neighborhood. Modeling of the gas sorption process by coal particle was carried out. To organize this kind of evolutionary process, the method of cellular automata modeling was supplemented by the Monte Carlo method to implement the boundary conditions at the solid – gas interface.

1 Introduction

When studying dispersed systems, it is necessary to take into account their internal properties. The main internal properties are: medium morphology, nature of gas interaction with the pore walls and the medium, which can be porous materials. Their consideration of as continuous media characterized by a certain coefficient of porosity does not satisfy the real picture of the materials under study, including gas-coal solution.

The problem is the use of mathematical models based on differential equations in partial derivatives to represent the material morphology at the microlevel and simulate the gas passage through the pores and thickness of the material [1], since the description by continuous functions of the pore boundaries is difficult, for example, when solving a parabolic equation describing diffusion in the area with a complex boundary.

The computing power of modern supercomputers makes it possible to solve this problem, for example, cellular automata are widely used to simulate diffusion processes, with the help of which some problems of gas dynamics have already been solved [2].

The objective of the research is the formation and application of cellular automata for modeling the movement of gas in materials with a complex boundary (porous medium).

Therefore, this article proposes a cellular automaton, the configuration of which imitates two types of movements of abstract particles in a porous medium: diffusion (spreading) and interaction with walls (equilibrium sorption).

2 Object of the study

The unloaded deep coal seam with an adjacent working is a gas-bearing porous system (dispersed system) with closed pores. This system consists of a solid medium (gas-coal

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solution) and a free gas phase in the pores. The coal substance of such a seam accumulates methane in various forms: gas in a free state inside the continuity defects (pores) – 2-12%; gas adsorbed on the surfaces of continuity defects – 8-16%; gas distributed in the intermolecular space (gas-coal solution) – 70-80%; chemically sorbed gas 1-2%; gas in clathrate-like structures – 1-3% [3]. The object of the study is the final volume of coal, in which the diffusion processes in a solid and equilibrium sorption take place at the solid-free gas interface, and is characterized by a uniform micropores distribution.

3 Cellular automaton modeling

The cellular automaton (CA) can be thought of as a stylized world in which space is represented by a uniform mesh, and each cell is encoded by a finite number of bits, time is discrete [4]. The laws of the transition of cell states determine the state of each cell at the current step by its state and the state of its neighbors at the previous step in time. Neighboring cells form its neighborhood [5]. That is, the rules of evolution (CA) are formulated in terms of local interaction using the von Neumann or Moore neighborhood. Let us define another class of CA – CA with Margolus neighborhood [5]:

1) the array of cells is divided into many finite parts - blocks;

2) a rule for a block is set, the rule is applied to all blocks, blocks do not intersect;

3) the division into blocks changes from step to step so as to ensure the intersection of blocks at adjacent steps.

Using the partitioning scheme: we divide the array of cells into 2x2 blocks – at even and odd time steps, two different divisions into blocks are made. In Fig. 1 the even lattice is shifted relative to the odd one by one cell vertically and horizontally. CA with Margolus neighborhood can be transformed into an ordinary CA.

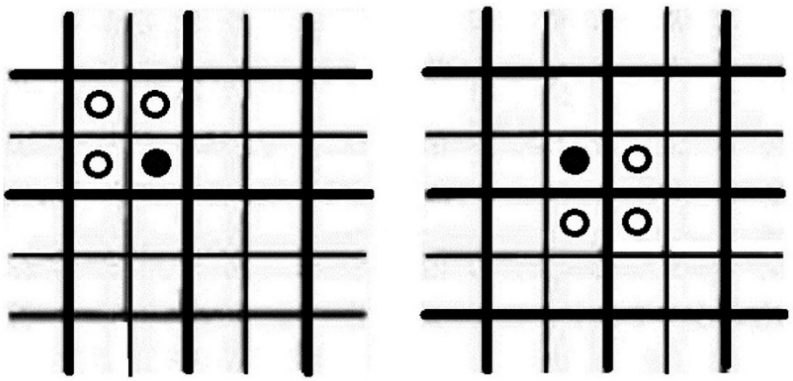

Fig. 1. Blocks 2x2 of Margolus neighborhood; even (bold lines) and odd lattices (thin lines) alternate in successive steps. Depending on the lattice used, a cell with a black circle will have either an even block or an odd block in its neighborhood.

Let us consider a model of gas sorption kinetics in the finite volume of coal. The sorption isotherm is described by the Langmuir equation. Gas transfer within a finite volume of coal is carried out by diffusion according to Fick's law.

Mathematical formulation of the corresponding two-dimensional problem [6]:

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right), \quad (1)$$

$$C(x, y, t_0) = C_0(x, y), \quad (2)$$

$$C(x, y, t) = \frac{abP(t)}{1+aP(t)}, \ (x, y) \in G, \quad (3)$$

where C is the concentration of the sorbed gas; D is the diffusion coefficient; P is the gas pressure; C_0 is the initial concentration value; a, b – coefficients of the Langmuir equation; G – particle surface.

We will proceed from the fact that gas diffusion in a porous solid is equivalent to self-diffusion. Consider the motion of an individual gas molecule. The collision of this molecule with other molecules leads to the fact that its motion has a stochastic character. Let us replace a real molecule with a lattice gas molecule that moves in jumps of unit length at discrete times along the infinite lattice with square cells. At each moment of time, all four directions of motion for a particle are equally probable. This model of particle motion is a random walk [7].

The essence of the lattice model of adsorption is as follows. There is a lattice of a finite number of centers, and all centers are the same. Each center can be in two states: the center is free; the center is occupied by an adsorbate molecule. The number of adsorbed molecules corresponds to the number of occupied centers. If we do not take into account the interactions between the occupied centers, then the mathematical description of the model results in the Langmuir equation [8].

The Langmuir equation in its lattice form determines the number of occupied adsorption centers as a function of gas pressure. This equation can be used as a criterion for discrete sorption equilibrium when setting boundary conditions of the form (2), (3) for a CA.

An essential part of the problem (1), (2), (3) set from the very beginning is the implementation of boundary conditions (2) and (3), which for cellular automaton can be carried out proceeding from the lattice model of adsorption [8], where a complex adsorption the surface field is replaced by a discrete one.

Random walk describes diffusion well [4]. The probability distribution for the random walk model is reduced to the distribution for the continual motion of a real molecule. The corresponding result was obtained analytically [7, 9, 10]. This was demonstrated for a two-dimensional CA [10]. Such a two-dimensional random walk is very efficiently implemented in the form of a CA with Margolus neighborhood.

A number of the most famous CA diffusion models are described in [11]. A rigorous proof of the correspondence of the CA-representation of diffusion to the Laplace differential equation is given in [12] for a CA with Margolus neighborhood. In the same place, for the first time, the value of the diffusion coefficient $D = \tau d/h^2$ was obtained for this CA model, which in the two-dimensional case is $D_{2D} = 3/2$. Further, this model will be described and used for the solution.

Algorithm of the functioning of a cellular automaton for studying the gas release kinetics is as follows. On the cell mass, two types of cells are distinguished: solid cells (coal particle) and free gas cells. Cells can be in one of two states: filled with a gas molecule and empty. The cells of free gas will be considered to be in an indefinite state: each of them contains a gas molecule with a certain probability. This probability is common for the entire array of free gas cells and is analogous to the free gas pressure (5).

The renewal of the state of cells in a solid is carried out in accordance with the rule for Margolus neighborhood (4). At the solid – gas interface, when dividing into blocks, cells of both phases fall into one block. When such a block is rotated, the gas molecule has the ability to leave the solid. The indefinite content of the free gas cell turns out to be on the solid-gas interface. It is necessary to correlate them in such a way that the relative number of border cells in the sorbent zone occupied by molecules is equal to the ratio of the number of adsorbed molecules to the total number of lattice centers. Which will fulfill the boundary

conditions (2), (3). A gas molecule that leaves the solid is absorbed. The probability of the presence of a molecule in the cell that has penetrated into a solid is equal to a uniy.

A cellular automaton model with Margolus neighborhood of two-dimensional diffusion (1) with boundary conditions (2), (3) – CA with a set of names $M = \{(i,j): i = 0,1,\dots,g;\ j = 0,1,\dots,l\}$ and with the neighborhood pattern $T\{i,j) = \{(i,j),(i+1,j),(i+1,j+1),(i,j+1)\}$. The function $v(i,j)$ can be considered as a Boolean cellular array $\Omega_B = \{(v_m, m)\}$, in which the cell is a pair of symbols (v_m, m), where v_m is a state variable, and $m \in M$ is the name of the cell from the set of names M, denoted by a pair of coordinates (i,j) in the case of a 2D-Cartesian space, and in the general case by one symbol m. The range of values of the state variables $v_m \in B$, where $B = \{0.1\}$ is the alphabet of states.

The transition rules from state to state are probabilistic for a rigid body without boundary conditions (3) having the following form:

$$\{(v_0,(i,j)),(v_1,(i+1,j)),(v_2,(i+1,j+1)),(v_3,(i,j+1))\} =$$

$$= \begin{cases} \{(v_1,(i,j)),(v_2,(i+1,j)),(v_3,(i+1,j+1)),(v_0,(i,j+1))\}, & if\ rand < p_S, \\ \{(v_3,(i,j)),(v_0,(i+1,j)),(v_1,(i+1,j+1)),(v_2,(i,j+1))\}, & if\ rand \geq p_S, \end{cases} \quad (4)$$

where $rand$ is a random number in the interval $(0,1)$; $p_S \leq$ ½ is the probability of interaction of the cell $(v_0,(i,j))$ with the neighboring cells for a solid body. At $p_S = 1/2$, the diffusion coefficient is $D = 3/2$. The CA operating mode is synchronous push-pull. At the first step, substitution (4) is performed by all cells with names satisfying the condition: $i + j$ is an even number. At the second stage, the same substitution is performed by cells for which $i + j$ is an odd number. By changing the value of the probability p, it is possible to simulate the diffusion process with a coefficient in a wide range [13], i.e., with decreasing p, the coefficient D decreases proportionally.

The transition rules from state to state are probabilistic for a free gas:

$$v_m = \begin{cases} 1, & if\ rand < p_G, \\ 0, & if\ rand \geq p_G, \end{cases} \quad (5)$$

where $p_G \leq$ ½ is the probability of filling the cell with a gas molecule $(v_0,(i,j))$ for the entire array of free gas. The higher p_G is, the higher the free gas pressure is.

4 Computational experiment results

The computational experiment is constructed as follows. The initial state of the system (CA) (2) is set, then the algorithm (4), (5) and the algorithm for the boundary condition (3) arising on the solid-gas interface are performed.

Fig. 2 shows the state of evolution of the process of gas sorption in a finite volume of coal containing four micropores with free gas. In the form of an initial state, characterized by the accumulation of gas along the left edge of the cell array in the solid and the hundredth step of the evolution of a given cellular automaton, characterized by a random, uniform distribution (spreading) of gas in the solid, which is the result of diffusion (random walk) of gas flowing in the solid (4). Cells in the pores with a certain probability, in our case 0.5, common for the entire part of the array occupied by pores, change their state: filled, empty (5). Equilibrium sorption occurs at the solid-free gas interface, expressed in the preservation of the initial state of the cell at this border. A two-dimensional model of a cellular automaton with Margolus neighborhood is used. The size of the cell array is 16x16

cells, which contains four 4x4 areas with free gas. Condition (3) was applied at the solid – gas interface. Cells with thick black borders are solid, cells with thin borders are solid – gas, cells with pale gray borders are free gas. Gray cells – the presence of a gas molecule (filled), white cells – the absence of a gas molecule (empty).

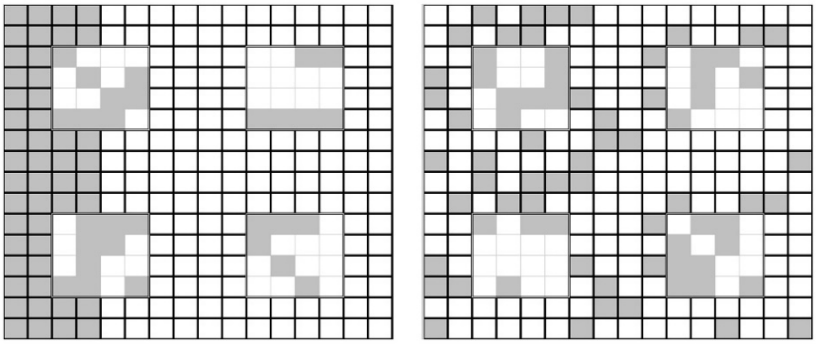

Fig. 2. Evolution states of the gas sorption process in the finite volume of coal: initial state; hundredth step

4 Conclusion

The corresponding algorithm is applicable for studying other physical processes, heat and electrical conductivity, magnetic and electromagnetic flows, etc. In such computer experiments, self-organization of matter is observed, and this self-organization follows from local interactions, the rule of which is set, and the structure arises itself.

Thus, the results of the performed numerical experiments have shown that cellular automata have a number of possibilities from the point of view of qualitative modeling of gas-dynamic processes. The developed methodology for computer modeling of the finite volume of coal provides for the use of a cellular automaton as a research tool. It consists in creating an algorithm and its computer implementation for studying the CA evolution, revealing the properties of the final volume of coal and their analysis.

The proposed cellular automaton is designed conceptually to simulate active media. It differs from the known cellular automata in that a cell has the same number of states for all, fixed for a specific evolution, the definition of which at each step is solved by the boundary diffusion problem, and a set of rules determines the state of each cell at the current step by the state of its and its neighbors at the previous step in time.

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