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CELLULAR AUTOMATA SYSTEMS APPLICATION FOR SIMULATION OF SOME PROCESSES IN SOLIDS

ZASTOSOWANIE AUTOMATÓW KOMÓRKOWYCH DO SYMULACJI NIEKTÓRYCH PROCESÓW W CIAŁACH STAŁYCH

Abstract

The article is devoted to the application of the discrete dynamical models for the study of some basic chemical processes. Basic approaches and general methodology for developing models based on cellular automata are considered by the examples of heat and mechanical energy transport processes. It is shown that in some cases these models can be an alternative to the application of classical differential equations.

Keywords: cellular automata, mathematical simulation, heat transfer, elastic deformation

Streszczenie

Artykuł poświęcony jest zastosowaniu dyskretnych modeli dynamicznych do badania wybranych procesów inżynierii chemicznej. Podstawowe metody i ogólną metodologię stosowania automatów komórkowych przedstawiono dla wybranych procesów wymiany ciepła i pędu. Wykazano, że w niektórych przypadkach modele te mogą być alternatywą dla stosowania klasycznych modeli opartych o równania różniczkowe.

Słowa kluczowe: automaty komórkowe, symulacja matematyczna, transport ciepła, odkształcenie sprężyste

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1. Introduction

The classical approach to the processes simulation in continuous environments using the fundamental transport equations and the equations of continuum mechanics is not always convenient. Parabolic and hyperbolic differential equations used require correct setting of several boundary conditions. Complexity increases when considering asymmetric areas or curved boundaries. Consideration using classical approaches of processes in isotropic materials as well as in the presence in the environment of the zones with different physical characteristics becomes extremely difficult.

These problems significantly limit the application of continual analytic approaches to studying basic processes of chemical technology. The application of numerical (finite difference) methods in the classical formulation is also difficult, and may not always be realized. The application of discrete dynamical systems and, in particular, cellular automata may be one of the directions of these processes simulation.

2. The concept of cellular automata

A cellular automaton consists of a set of discrete elements (cells) which form a spatial lattice. In general, lattices may be different both in dimension and shape of cells. Each cell operates under the laws of abstract automaton. Therefore, it can be represented as a "black box" that may have some internal states, to which input signals are transmitted and output signals are read off. The main feature of a cellular automaton is that its behavior is completely determined by local interaction of its elements.

Considering the operation of individual cell in terms of the finite automata theory it is necessary to suppose the following. Each cell is connected by its inputs to the outputs of neighboring elements. The output of each element is an input for the neighboring cell. Each individual cell is an object that operates in discrete time $t_0 < t_1 < t_2 < \ldots$ At any time point t_i the cell is in one of the potential states $z(t_j)$ and its inputs can receive input signals $x(t_j)$. With their input the cell state varies according to the one-step transition function:

$$z(t_j) = \varphi[z(t_{j-1}), \bar{x}(t_j)] \tag{1}$$

In simulation practice there also can be used multi-step transition functions, which in contrast to (1) include the prehistory of the automaton:

$$z(t_j) = \varphi\{[z(t_{j-1}), z(t_{j-2}), \ldots,]\bar{x}(t_j)\} \tag{2}$$

In general, systems of cellular automata are characterized by the following properties [1, 2]:

1. The state space of the system is discrete.
2. The states of all cells in the system are changed at the same time by the same rules.
3. Particular cell can be influenced by neighboring cells only.

The last property is very important while simulating the transport processes. It shows that the behavior of cellular automata is fully determined by local interactions of their elements. The case is the same for a large class of continuous dynamical systems described by partial differential equations. This makes it possible to recommend the cellular automata to model the transport processes of matter and energy.

3. Application of cellular automata for simulation of dynamic systems

Let us consider the basic approach and a common methodology for simulation application of cellular automata [4].

First of all, the continuous model space is divided into cells (elements) on the functional basis. Partitioning can be uniform with obtaining the same elements, but it is not necessary, and it is often done only for the convenience of simulation. The main purpose of space discretization is to obtain such cells of the space within which it is functionally homogeneous. Sizes of these cells must be such that the parameters of the processes inside them can be regarded independent of spatial coordinates. In this case the only independent variable for describing the behavior of each cell is time.

Next, it is worth to describe the behavior of cells by means of expressions (1) ÷ (2), considering that the state of the cells is a discrete space-time function. For this purpose general laws of the process under investigation are used. It is advisable to take the intensive phase variables of the corresponding process (temperature, concentration, speed, etc) as the states of the cells. In this case output signals of the cell (the automaton) will be extensive state variables – heat flow, mass flow, mechanical strength, etc. Thus, after discretization of the space one will obtain the interrelated array of cells the behavior of which over time (in this case, discrete) will be subjected to the laws of the simulated process.

It should be noted that functions (1) ÷ (2) used here must not always be determined and in some cases may have a probabilistic nature.

4. Simulation of one-dimensional heat conduction problem

Let us consider the one-dimensional body of finite length, consisting of the elements of the same size h (Fig. 1). In this case the internal elements are connected with two neighboring ones, and the cells located at the borders will have one neighboring that.

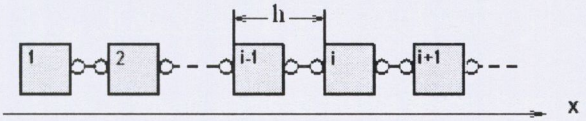

Fig. 1. The scheme of one-dimensional cellular automaton model of heat transfer within the molecular mechanism

Rys. 1. Schemat jednowymiarowego automatu komórkowego dla molekularnego mechanizmu przenikania ciepła

State of the element (cell) for a given physical system simulates its temperature. Signals the cell – automaton simulate the transfer of heat between the system elements. Therefore, the output signals of the element i will be the input for the elements i-1 and i+1. Therefore, the state change function of each cell can be written as (1) like that

$$T(t_{k+1}) = F[T(t_k), \sum_{j=1}^{n} q_j(t_k)] \tag{3}$$

where T is temperature, °C; q is specific heat flux, W/m^3; n is the number of cell-automaton inputs. Getting a specific form of the dependence (3) is possible by using the following well-known principles of physics.

According to the law of the Fourier heat flux vector (quantity of energy passing in unit time through unit area) is proportional to the temperature gradient. In considering each cell as parallelepiped one can write the law of heat conduction in the integral form as follows:

$$q = \frac{\lambda \cdot \Delta T}{h^2} \tag{4}$$

where λ – coefficient of thermal conductivity, W/(m·°C); h – length of the parallelepiped (step along the coordinate), [m].

Let us consider the heat balance of the i-th cell at time k.

The specific heat flux from cell i to cell $i+1$ for time step k in the discrete model can be written as:

$$q_{i,i+1}(t_k) = \lambda_i \frac{[T_i(t_k) - T_{i+1}(t_k)]}{h^2} \tag{5}$$

where $q_{i,i+1}(t_k)$ – heat flux from cell i to cell $i+1$; λ_i – thermal conductivity of the cell i environment; $T_i(t_k)$ and $T_{i+1}(t_k)$ – temperature of cells i and $i+1$ at time k.

The specific heat flux from cell i-1 cell i:

$$q_{i-1,i}(t_k) = \lambda_{i-1} \frac{[T_{i-1}(t_k) - T_i(t_k)]}{h^2} \tag{6}$$

where λ_{i-1} is thermal conductivity of the cell i-1 environment.

Thus, the heat balance of the i-th cell:

$$\begin{aligned} &\sum q_i(t_k) = q_{i-1,i}(t_k) - q_{i,i+1}(t_k) + \gamma(t_i) = \\ &= \left[\lambda_{i-1} \cdot \frac{[T_{i-1}(t_k) - T_i(t_k)]}{h^2} - \lambda_i \cdot \frac{[T_i(t_k) - T_{i+1}(t_k)]}{h^2} + \gamma(t_i) \right] \end{aligned} \tag{7}$$

where $\gamma(t_i)$ is power density of heat sources located in the cell i, W/m^3;.

Transition function (3) for the considering processes can be explicitly written as follows:

$$T_i(t_{k+1}) = T_i(t_k) + \frac{\Delta t}{C_i \cdot \rho_i} \cdot \sum q_i(t_k) \tag{8}$$

where C_i is specific heat capacity of i-th cell material, J/(kg·°C); ρ_i is its density, kg/m^3; Δt – time step, s.

Reasoning similarly and giving the conditions at the boundaries of the modeled area it is easy to obtain similar expressions for the cells at the boundary of the area.

Thus, we obtained local rules that allow determining the new state of each element of the cellular automaton for each time step and make it possible to simulate one-dimensional heat transfer process with a certain initial temperature distribution. Allowance of external

threads and internal heat sources can be accomplished by introducing the necessary specific values of temperature and flows for the corresponding elements of the modeled system. The process of the thermal conductivity simulation is reduced to the determination of cellular automaton elements states at each stage of discrete time using expressions (5) ÷ (8).

Now let us consider the one-dimensional non-stationary problem of heat conduction, where the object will be a uniform rod of finite length divided into 41 cells. Physical properties of the rod material are the specific heat capacity of 700 J/(kg·°C), density of 1300 kg/m^3. Parameters of simulations: spacing along the coordinate makes 1 mm, the time step makes 0.1 s. It was assumed that in the middle of the rod (cell 20) at the initial time heat momentum magnitude of 300 °C and duration of 1 model time step. The simulation process is reduced to the determination of the cells states at each time step. In this case it was used the transition function of the form (5) ÷ (8) for internal cells, and for boundary cells these dependences are modified based on the hypothesis of zero temperature gradient in the boundary points (the equality of heat flows from the neighboring cells).

As an Example 1 let us take a simple case of heat transfer at a constant thermal conductivity (linear problem) and the absence of internal heat sources. The results are shown in Fig. 2. The value of thermal conductivity was assumed to be 2.5 W/(m·°C).

Data analysis shows that the heat is distributed along the rod from the warmer areas to the less heated and the temperature (in the limit) tends to a steady value. It is a well-known picture of the thermal conductivity.

To complicate the problem we consider Example 2, where we have the effect of temperature on the value of thermal conductivity and an internal heat source with a non-linear power change law. We assume the following [5].

$$\gamma(T) = k \cdot T \cdot \beta \tag{9}$$

$$\lambda(T) = \lambda_0 \cdot T \cdot \alpha \tag{10}$$

Illustration of Example 2 with $k = 0.6$; $\beta = 1.3$; $\alpha = 0.1$ is given in Fig. 3.

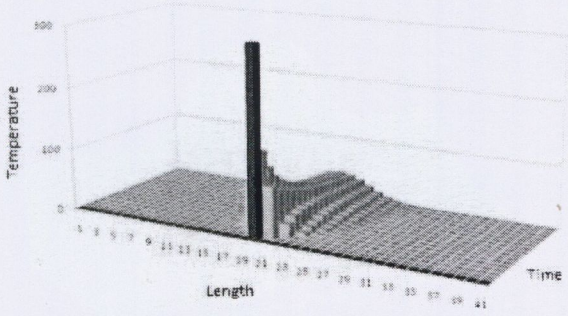

Fig. 2. The change of the temperature in Example 1

Rys. 2. Zmiana temperatury – przykład 1

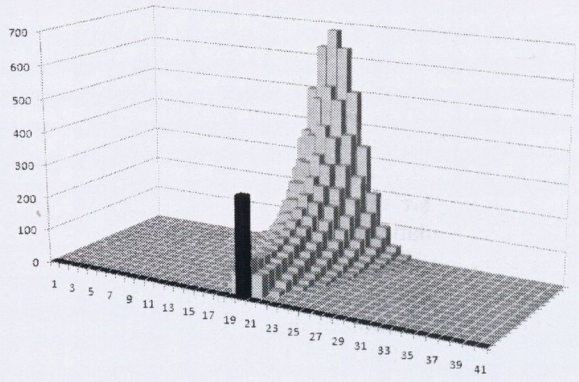

Fig. 3. The change of temperature in Example 2

Rys. 3. Zmiana temperatury – przykład 2

One may notice that the temperature in the central zone increases sharply and, what is more important, heated areas are located and formed the temperature torch.

It should be said that the example can illustrate the process of burning, but only in the initial stages, as an unlimited increase of temperature contradicts the physical picture of the real process.

Let us investigate the process considering endothermic effects, which are often presented in the real world. In Example 3 we introduce the following law of dependence between source specific power and temperature:

$$\gamma(T) = k \cdot T - \gamma \cdot T^3 \tag{11}$$

Effect of temperature on the transport coefficients change will be consider by the expression (10). The simulation results for $k = 0.25$; $\gamma = 0.01$; $\alpha = -0.5$ are shown on the Fig. 4.

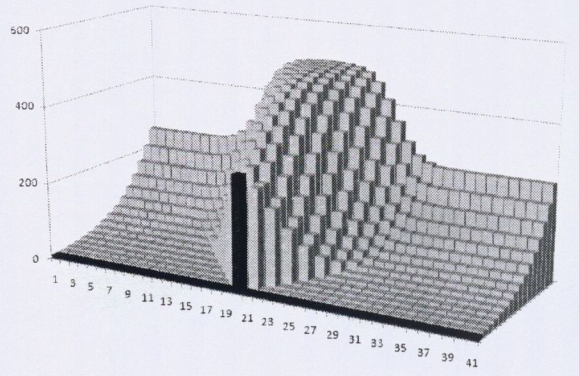

Fig. 4. The change of temperature in Example 3

Rys. 4. Zmiana temperatury – przykład 3

These data differ significantly from those given above. First of all, it is evident that the temperature in the central region tends to a limiting value, and the distribution of heat has a form similar to the wave, since it has quite a pronounced front. In real processes, this situation can occur, for example, fuel burn up. It may be noted that these results obtained using the discrete dynamical model are consistent with classical concepts on the flow of these processes.

It is not difficult to extend the proposed methodology to two- and three-dimensional space. In addition, this approach allows simulating the process in the objects of complex shape with curved surfaces.

It should also be noted that deep analogy between the processes of heat and mass transfer allows the use of the considered approach to modeling of diffusion processes.

5. Simulation of elastic solid deformation

Let us consider the simplest one-dimensional model of an elastic solid, which in general is not homogeneous. Imagine a solid body as a chain of N unit cells of linear size h, each of which has mass and elasticity (Fig. 5).

While formulation the problem in question, cell-automaton state is simulated by the deformation (shift). The signals of neighboring automata simulate energy transfer process of mechanical action between the elements of the system. What distinguishes this case from the heat transfer considered above is the existence of a more complex function to calculate the states of cellular automata. Since the process of energy transfer of mechanical momentum is a wave shaped, the elements that simulate the behavior of the system should have a "memory", i.e. they should be automata with aftereffect.

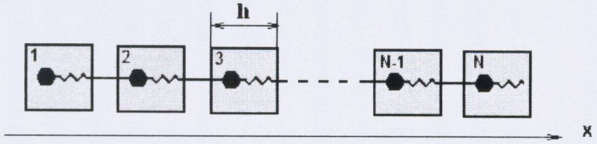

Fig. 5. The scheme of one-dimensional cellular automaton model of an elastic body

Rys. 5. Schemat jednowymiarowego automatu komórkowego dla ciała sprężystego

Therefore, the functional relationship for the calculation of the subsequent state will have the form (2), since there must be considered not only a current state but also a previous one:

$$u(t_{k+1}) = F[u(t_k), u(t_{k-1}), \sum_{j=1}^{n} x_j(t_k)] \tag{12}$$

where u is cell shift, m; x is variable, which takes into account the flow of elastic energy from neighboring cells.

Take into consideration u – cells deformation of the model of mechanical stress on the body, provided that $u << h$ (Fig. 6).

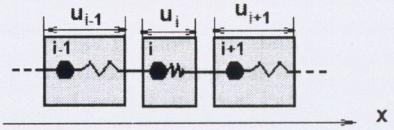

Fig. 6. Deformation of the *i*-th element

Rys. 6. Odkształcenie *i*-tego elementu

Mechanical stress in the *i*-th cell expressed in terms of absolute deformations (shifts) of neighboring cells, for time step *k* will be of the form:

$$\sigma_i(t_k) = E_{i+1} \cdot \frac{u_{i+1}(t_k) - u_i(t_k)}{h} + E_{i-1} \cdot \frac{u_{i-1}(t_k) - u_i(t_k)}{h} \tag{13}$$

where σ is mechanical stress, Pa; E is modulus of elasticity of the element material, Pa; h – step of the space discretization, m.

At the same time, one can write the following expression for the mechanical stresses in integral form:

$$\sigma = \frac{m \cdot a \cdot h}{V} = a \cdot \rho \cdot h \tag{14}$$

where m is mass of cell, kg; V is volume of cell, m^3; a is acceleration of the cell mass centre, m/s^2.

Therefore from (13) and (14) one can get:

$$a_i(t_k) = C_{i+1}^2 \cdot \frac{u_{i+1}(t_k) - u_i(t_k)}{h^2} + C_{i-1}^2 \cdot \frac{u_{i-1}(t_k) - u_i(t_k)}{h^2}$$

$$C_i = \sqrt{E_i / \rho_i} \tag{15}$$

where C is speed of elastic waves in the material of cell, m/s.

If one assumes that u is discrete function of not only the coordinates x, but also the time t, then the expression for the transition (12) can be written explicitly:

$$u_i(t_{k+1}) = 2 \cdot u_i(t_k) - u_i(t_{k-1}) + \Delta t^2 \cdot [p_{i+1}(t_k) + p_{i-1}(t_k)]$$

$$p_{i+1}(t_k) = \frac{C_{i+1}^2 \cdot [u_{i+1}(t_k) - u_i(t_k)]}{h^2} \qquad p_{i-1}(t_k) = \frac{C_{i-1}^2 \cdot [u_{i-1}(t_k) - u_i(t_k)]}{h^2} \tag{16}$$

In the analysis of the expression (16) one should aware that the variable p can be interpreted as the value of the neighboring cell force impact per unit mass.

The dependences obtained are local rules allowing to determinate the new state of each cell for each time step. Reasoning similarly one can obtain equations of conduct outer (boundary) elements of the system. The external pressure is considered by introducing the necessary concrete strain values (state) for one of the boundary elements of the system.

Let us show the applicability of the proposed approach. First we consider a trivial problem of momentum propagation in an isotropic thin rod. Take the rod of length 10 mm from material having an elastic wave velocity of $C = 5000$ m/s, and divide it into 10 elements with a step $h = 1$ mm. Set time step $\Delta t = 0.2$ μs. To simulate the external influence on the first (leftmost) element let set change of its deformation in the form of a single momentum a time step duration and amplitude of 0.5 μm. For clarity, we assume a rectangular momentum shape.

Fig. 7 shows the simulation results in form of components i deformation values u for the different moments of time k.

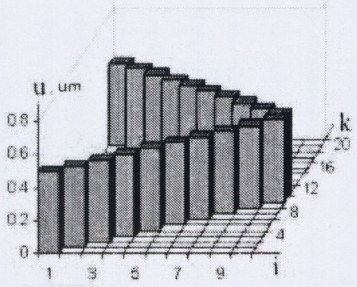

Fig.7. Momentum deformation movement along the rod

Rys. 7. Transport odkształcenia wzdłuż pręta

One can see that momentum is moving along the rod, reflecting from its ends and moving in the opposite direction. This picture is consistent with the generally accepted ideas. Since the material of the rod is taken ideal, momentum shape is not distorted and the movement continues in time forever.

Let us turn to two-dimensional model. Imagine a solid as an array of $M \times N$ elements of size $\Delta x \times \Delta y$, each of which has mass and elasticity. Fig. 8 shows the scheme of the discrete two-dimensional model of the solid.

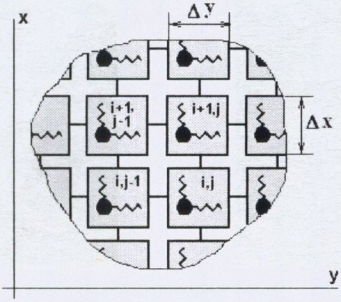

Fig. 8. The scheme of two-dimensional cellular automaton model of an elastic body

Rys. 8. Schemat dwuwymiarowego automatu komórkowego dla ciała sprężystego

When considering the deformation process of two-dimensional body in a first approximation we can consider the case of a uniaxial deformation. This allows to assume that the impact on the body and, consequently, the deformation of the elements will be directed strictly along one axis. Solving this problem one should aware that in this case the two elastic waves – longitudinal and transverse – covered in the material. The approach enables to obtain expressions for the simulation of each of the waves, which are formally similar to equations (16). Using the superposition principle of waves, the total deformation can be represented as the sum of the deformation caused by each wave separately.

The transition function (local rules) for the element with the indices i, j will be:

$$u_{i,j}(t_{k+1}) = 2u_{i,j}(t_k) - u_{i,j}(t_{k-1}) + \Delta t^2 \left[p_{i+1,j}(t_k) + p_{i-1,j}(t_k) + p_{i,j+1}(t_k) + p_{i,j-1}(t_k) \right]$$

$$p_{i+1,j}(t_k) = \frac{C^2_{i+1,j}(x)[u_{i+1,j}(t_k) - u_{i,j}(t_k)]}{\Delta x^2} \quad p_{i-1,j}(t_k) = \frac{C^2_{i-1,j}(x)[u_{i-1,j}(t_k) - u_{i,j}(t_k)]}{\Delta x^2}$$

$$p_{i,j+1}(t_k) = \frac{C^2_{i+1,j}(y)[u_{i,j+1}(t_k) - u_{i,j}(t_k)]}{\Delta y^2} \quad p_{i,j-1}(t_k) = \frac{C^2_{i,j-1}(y)[u_{i,j-1}(t_k) - u_{i,j}(t_k)]}{\Delta y^2} \tag{17}$$

where $C_{i,j}(x)$ is elastic wave velocity in the direction of the x-axis; $C_{i,j}(y)$ is the same in the direction of the y-axis.

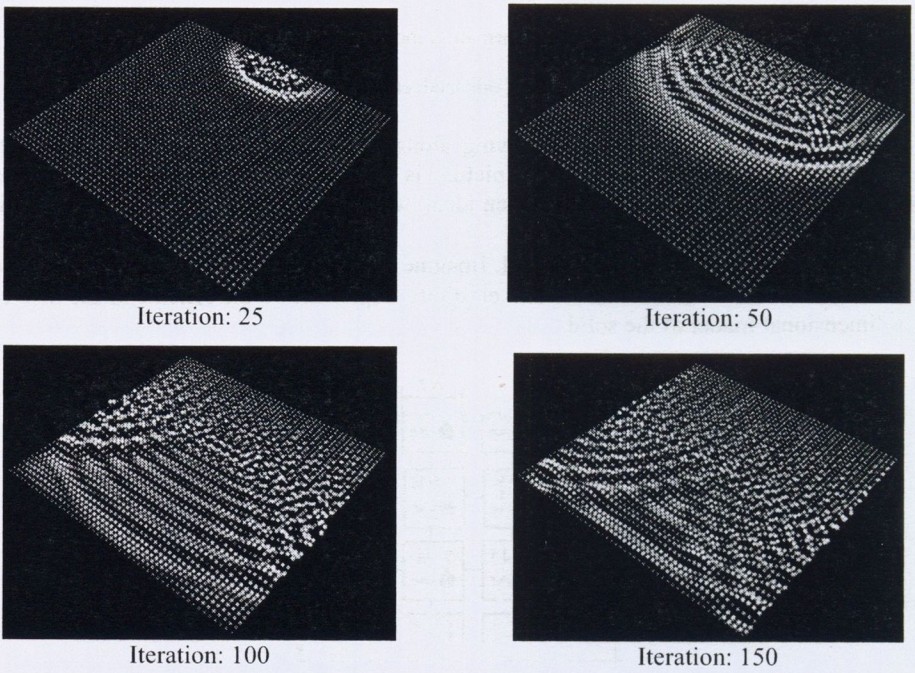

Fig. 9. The deformation picture in the plate at different times

Rys. 9. Zmiana deformacji płyty w czasie

Below there are the results modeling of elastic wave propagation in a flat square-shaped body. In simulation the main parameters was following: the size of the plate was 10×10 mm, the velocity of propagation of elastic waves in longitudinal and transverse directions was assumed the same and equal to 5000 m/s, time step duration was $2 \cdot 10^{-8}$ s, step in the coordinates was 0.2 mm.

When simulation a periodic forcing on one of the cells located at the edge of the plate was simulated. The results are listed in fig. 9. The cell deformation value was coded by brightness of the corresponding point.

The results obtained show that in the process of propagation of elastic waves they reflect from the edges of the plate increase and decrease each other; that corresponds to the current views on the nature of the process.

6. Conclusion

Mathematical simulation of real processes can be performed using different approaches and models. The author by no means to oppose the proposed approach to continuous deterministic models based on differential equations. However, differential equations are well known to be based on mathematical infinitesimals, which are a mathematical abstraction. At the same time in nature there is no infinitesimals, but there are physical quantities that can be extremely small, but remain finite. As the study of the microscopic level and nano-level phenomena it is clear that such phenomena are not always sufficiently well described by differential equations, and often require the application of other modeling principles.

In the early development of the cellular automata theory attempts to use them to solve differential equations were made. In this paper we consider the opposite approach – it is shown that the transition function of cellular automata can be obtained using the rules of local interaction and simple balance equations of the process. In turn, in particular cases, these transition functions are identical to finite-difference analogues of the classical transfer equations.

Thirty years ago, Academician A. N. Kolmogorov predicted that with the development of modern computer technology it often will be wise to study real phenomena avoiding the intermediate step of their stylization in the frameworks of mathematics of the infinite and continuous, and will move straight to the discrete model [3]. Now, with the advent of powerful computer support one can state that this prediction of the great Russian mathematician comes true.

Literature

[1] Wolfram S.: *Theory and applications of cellular automata,* Singapore: World Scientific, 1986.

[2] Toffoli T., Margolus N.: *Cellular Automata Machines*. Cambridge, Massachusetts: The MIT Press, 1987.

[3] Kolmogorov A. N.: *Mathematics – the science and profession*. M.: Phiz.-math. lit. 1988.

[4] Bobkov S. P.: Izv. Vyssh. Uchebn. Zaved. Khim. Khim. Tekhnol., V. 52. N 3, (2009), 109-114.
[5] Bobkov S. P., Voitko J. V.: Izv. Vyssh. Uchebn. Zaved. Khim. Khim. Tekhnol., V. 52 N 11, (2009), 126-128.