The use of cellular automata systems for simulation of transfer processes in a non-uniform area

Sergey Bobkov, Edward Galiaskarov and Irina Astrakhantseva

Ivanovo State University of Chemistry and Technology, 7, Sheremetevskiy Avenue, Ivanovo, 153000, Russian Federation
galiaskarov_eg@isuct.ru

Abstract. The article is devoted to the issues of using discrete dynamic models as an alternative to the classical methods of studying the basic processes of chemical technology. An adequate description of the phenomena of transfer of matter and energy is an extremely important task, both in theoretical terms and from the standpoint of their practical use. Studies of real processes using the equations of mathematical physics have shown that they allow correctly describing real processes only in homogeneous media and only under conditions closing enough to equilibrium. When modeling processes in heterogeneous environments, as well as when considering significant external influences, computational difficulties arise. The fundamental opposite of classical modeling methods should be considered approaches that use local sampling of the process under consideration, in particular, systems of cellular automata. The paper considers the capabilities of discrete dynamic models based on deterministic cellular automata. Models allow us to consider space as a combination of separate interconnected elements, the behavior of which obeys local rules. The basic techniques and general methodology for the development of discrete models are presented. Examples of their use for modeling heat conduction and diffusion processes are given, taking into account the non-uniform of the material and the presence of volumetric sources. The data obtained do not contradict the data obtained by classical methods and the principles underlying the theory of transport phenomena.

Keywords: Discrete modeling, Cellular automata, Thermal conductivity, Diffusion, Nonlinear problems of substance transfer.

1 Introduction

Classical approaches to modeling the basic laws of transfer of matter and energy involve the use of partial differential equations [1-2]. Despite the significant contribution to the creation and development of engineering science, at present, the shortcomings of classical equations are increasingly noted [3]. These shortcomings

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are based on the fact that the classical equations, being continual, consider the processes of mass and energy transfer in a continuous homogeneous medium and use constant transport coefficients (diffusion, thermal conductivity, etc.). These assumptions, as practice has shown, often lead to not entirely adequate results [4], especially in cases where:

- The properties of the environment are not constant in time and space;
- The object of modeling has a complex shape and curvilinear boundaries;
- The presence of discontinuous or threshold functions in the equations.

These problems can significantly limit the use of continuous models, which requires a wider use of discrete approaches, which include cellular automata models [5-6].

2 Materials and methods

2.1 Formalization of the cellular automaton

The system of cellular automata is a dynamic model that defines a continuous environment in the form of a combination of discrete elements - cells, each of which is an abstract automaton. Within the framework of the theory of automata, a cell is defined as an object that can change its states under the action of input signals. The change of states is specified, as a rule, by a deterministic transition function φ. That is, the state of the automaton $z(t_{k+1})$ at time $k+1$ is a function of only two variables: the state $z(t_k)$ and the input signal $x(t_k)$ at the previous time k. Consequently, an automaton cell is an object that operates in discrete time steps $t_0<t_1<t_2<\ldots, t_k$. This makes it possible to describe the change in its state over time. Individual cells form a spatial lattice, the dimensions and shapes of which, in the general case, are arbitrary [7-8].

When passing from an individual cell to a set that makes up a system of cellular automata, the problem arises of determining the set of cells that fill the model space and describing the connections between cells. In cellular automata for modeling two-dimensional processes, you can define a cell using its coordinates. Connections between cells can be introduced as follows. It is considered that each automaton cell has inputs, which are outputs of other cells - neighbors. At the same time, the neighbors are located in a certain limited neighborhood. In two-dimensional models of cellular automata, two types of neighborhoods of cells are most often used: the von Neumann neighborhood and the Moore neighborhood [9-10]. Further in this paper, we will consider systems with a von Neumann neighborhood on a square lattice, which is a collection of four cells that have a common side with the cell under consideration. Let's denote the set of neighbors of the i cell as $O(i)$. Thus, if $j \in O(j)$, then the cell named j is a neighbor of the cell i.

Let us concretize the type of cellular automaton, for which we restrict ourselves to considering homogeneous deterministic elements of the system. Homogeneity means that all cells are equal and affect each other equally. Since the inputs of a particular cell are, in fact, the outputs of neighbors, it can be argued that the input signals of a

cell are the states of its neighbors. Thus, the transition function for a homogeneous deterministic cellular automaton will have the form:

$$z_i(t_{k+1}) = \varphi\left(z_i(t_k), \sum_{j \in O(i)} z_j(t_k) \right) \quad (1)$$

Transitions between states are carried out in steps of model time for all cells synchronously.

From expression (1) it can be seen that the rules of evolution of a system of cellular automata are local, since the state of each specific cell depends on the state of the nearest neighbors, and more distant cells do not have any effect on it.

2.2 General modeling methodology

Let us consider the main stages of applying the methodology for modeling substance transfer processes using cellular automata.

Sampling of the model space. At the first stage of modeling, the continuous space is divided into cells using some kind of spatial lattice, for example, orthogonal [5]. At the same time, there is a fundamentally important point - the size should be set in such a way that the parameters of internal processes do not depend on spatial coordinates. In addition, cell division allows you to investigate processes in objects with curved boundaries.

Further, in dependencies of type (1), it is required to indicate the explicit form of the functions φ. This allows you to establish a connection between external influences and the state of cells. The formalization of this connection is ensured by using the fundamental laws of a particular modeled process. For example, in the study of transfer processes, the state of cells can be compared with phase variables of a potential type. Temperature will play such a role for thermal processes, and component concentration for diffusion processes. As external influences (input signals), it is advisable to take flux quantities - heat flux, mass flux, etc. As a result, it is possible to obtain a cellular system, the behavior of which will obey the laws of a specific modeled process.

Derivation of the laws of cell functioning. To obtain the transition function (1) in an explicit form, the technique described in detail in [11] was used. The conclusion was based on the use of one of the forms of recording the laws of conservation of substance (energy, mass), according to which the flow of transfer of a substance is associated with a potential gradient. In the derivation, the specific (per unit volume) flows of a substance were considered, associated with the potential difference by transport (kinetic) coefficients. When specifying the flows of substance, it was assumed that the cells under consideration have a von Neumann neighborhood and exchange flows. As a result, an equation was obtained that is valid for describing the processes of transfer of energy or mass, which are carried out by the microscopic movement of particles of matter:

$$F_{i,j}(t_{k+1}) = F_{i,j}(t_k) + \frac{\Delta t}{h^2} \cdot \sum a_{i,j} g_{i,j}(t_k) \quad (2)$$

Where: $F_i(t_k)$ - state (potential value) of the i cell at the k time step; $F_i(t_{k+1})$ - the same at the k+1 time step; Δt - time quantization interval; h - step along spatial coordinates; $a_{i,j}$ - transport coefficient taking into account the properties of the material of the i cell; $g_{i,j}(t_k)$ is the flow of substance between neighboring cells in a discrete time step t_k.

Expression (2) allows you to analyze the dynamics of changes in the state of the cell in time.

It is easy to see that this approach allows you to simulate processes in an object, the physical properties of which are inhomogeneous. Indeed, the characteristics of the substance are included in the local dependence (2), which already makes it possible to take into account the spatial heterogeneity. If the properties of the material change over time, or depend on the state of the cell, then these effects can be taken into account using additional expressions.

The existence of special cells. It is easy to see that expression (2) will be valid both for inner cells surrounded by exactly four neighbors and for edge cells with less than four neighbors. In general, when using this expression, the presence or absence of exchange of a substance with the environment should be taken into account.

Situations are possible when it is necessary to simulate an object containing local sources or sinks of a substance, that is, zones where energy or mass is generated or absorbed. In this case, it is convenient to introduce an additional term into the expression for the transition function:

$$F_{i,j}(t_{k+1}) = F_{i,j}(t_k) + \frac{\Delta t}{h^2} \cdot \sum a_{i,j} g_{i,j}(t_k) + \Delta t \cdot \gamma(t_k) \qquad (3)$$

Where $\gamma(t_k)$ is the specific power of the source (drain) of the potential.

After the formation of an array of cells and determination of the laws of their functioning of the form (2) - (3), the values of the necessary constants characterizing the parameters of a particular process and the initial states of the cells should be set. The modeling process will consist in determining the values of the array elements for successive moments of discrete time.

3 Simulation results

3.1 Modeling the heat conduction process

Consider the process of heat transfer caused by microscopic (molecular) movement of matter - the process of heat conduction.

Concretization of the physical essence of the process allows us to indicate that the transported substance here will be heat energy. Therefore, in this particular case, the temperature should be taken as the transfer potential, which will correspond to the state of the cells of the automata system. Cells in the process of heat transfer will exchange flows of heat. A set of indicators of thermal conductivity, heat capacity and density of the cell material will act as the transport (kinetic) coefficient. In this case, the equation of the transition function (3) takes the form:

$$T_{i,j}(t_{k+1}) = T_{i,j}(t_k) + \frac{\Delta t}{h^2} \cdot \sum \frac{\lambda_{i,j}}{C_{i,j}\rho_{i,j}} g_{i,j}(t_k) + \Delta t \cdot \gamma(t_k) \quad (4)$$

Where $T_{i,j}(t_{k+1})$ and $T_{i,j}(t_k)$ are the cell temperature at times t_{k+1} and t_k; $\lambda_{I,j}$, $C_{i,j}$ and $\rho_{i,j}$ are the thermal conductivity, heat capacity and density of the material of the cell i, j, respectively.

Example 1. Consider an imitation of the combustion process. For this, we use equation (4), in which the specific power of the volumetric source is proportional to the temperature:

$$\gamma(T) = kT \quad (5)$$

Where k is a constant.

Thus, we arrive at a quasilinear problem in which heat transfer occurs under conditions of heat release.

As a model object, a plate was chosen, broken with a step of 1 mm into 1681 (41×41) cells. The following material characteristics were used: thermal conductivity 1.5 W / (m·K), specific heat 1000 J / (kg·K), and density 1500 kg / m^3. The constant k in expression (5) was equal to 0.025. The initial temperature of the plate was taken equal to 0 conditional degrees. The simulation step in time was 0.005 s. There was no heat exchange between the plate and the environment. Combustion was initiated by an instantaneous heat pulse in the center of the plate.

Figure 1 shows the simulation results. The abscissa and ordinate axes show the dimensions of the plate, and the applicate axis shows the temperature in arbitrary units. The physical time in seconds is indicated in the upper right corner.

Analysis of Figure 1 shows a picture typical in real conditions for the initial period of the combustion process. At first, the heat spreads over the plate rather slowly. And then, in the area of influence of the initial pulse, the temperature rises sharply.

Example 2. In order to demonstrate the capabilities of the discrete approach, let us consider heat transfer in an inhomogeneous material. Let's make the following changes to the previous task.

Let us assume that the investigated plate contains a section, the material of which has a much lower ability to conduct heat than the rest of the object's mass. For this, let us assume in equation (4) that the thermal conductivity of the anomalous section is two orders of magnitude lower than for the main part of the plate. Leave all other parameters of the problem unchanged.

The results are shown in Figure 2. As you can see, the temperature of the area with lower thermal conductivity stands out sharply against the general thermal field. In this case, the temperature of the anomalous area changes weakly with time, and the heating of the plate under study are noticeably slower than that observed in the previous example (Figure 1).

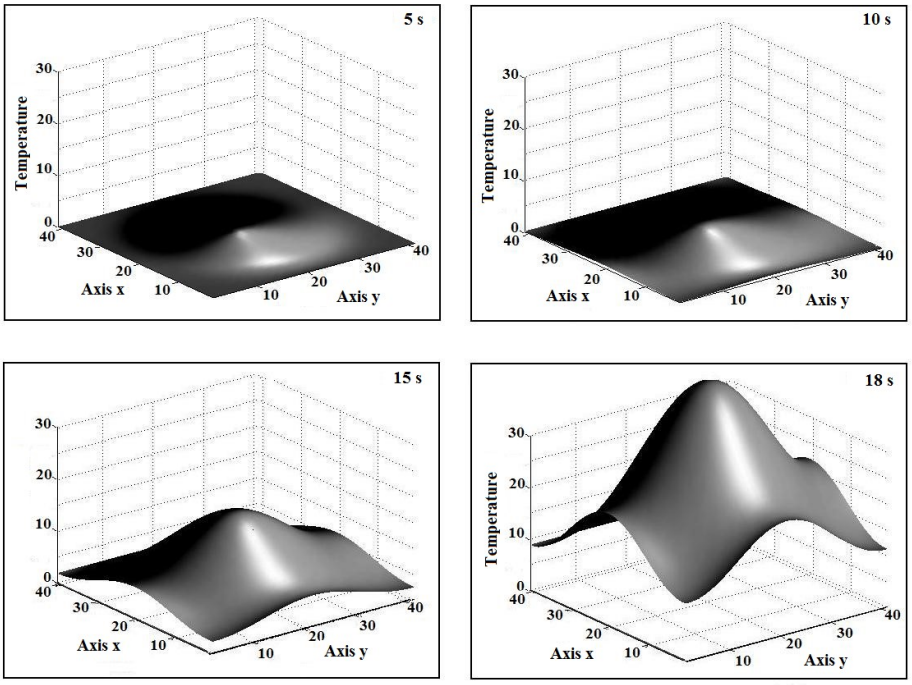

Fig. 1. Results of the study of the quasilinear model of thermal conductivity.

3.2 Simulation of the diffusion process

Let us turn to the consideration of the application of systems of cellular automata for modeling the mass transfer by the molecular mechanism. As a first approximation, we will assume that the process takes place in a single-phase system at a constant temperature and in the absence of external forces.

In this case, the laws of functioning of the cells of the automaton should take into account that the mass of the substance becomes the transferred substance. Hence it follows that the cells will exchange flows of mass, and concentration will act as the transfer potential. The transport coefficient in the above expressions (2) and (3) will be the molecular diffusion coefficient.

Now the equations of the transition function (3) can be written as follows:

$$M_{i,j}(t_{k+1}) = M_{i,j}(t_k) + \frac{\Delta t}{h^2} \cdot \sum D_{i,j} \cdot g_{i,j}(t_k) + \Delta t \cdot \gamma(t_k) \qquad (6)$$

Where $M_{i,j}(t_{k+1})$ and $M_{i,j}(t_k)$ is the concentration of the component in cell i,j at times t_{k+1} and t_k ; $D_{i,j}$ is the diffusion coefficient of the cell material.

Example 3. To illustrate the possibilities of equation (6), let us consider the imitation of the diffusion process in a two-dimensional object in the presence of mass sources in it. There was a rectangular plate divided into (21×31) cells with a step of

1 mm. The diffusion coefficient was taken equal to $0{,}1 \cdot 10^{-6}$ m^2 / s. The initial concentration of the substance in the plate is equal to 0 conventional units. The time sampling step corresponded to 0.2 s.

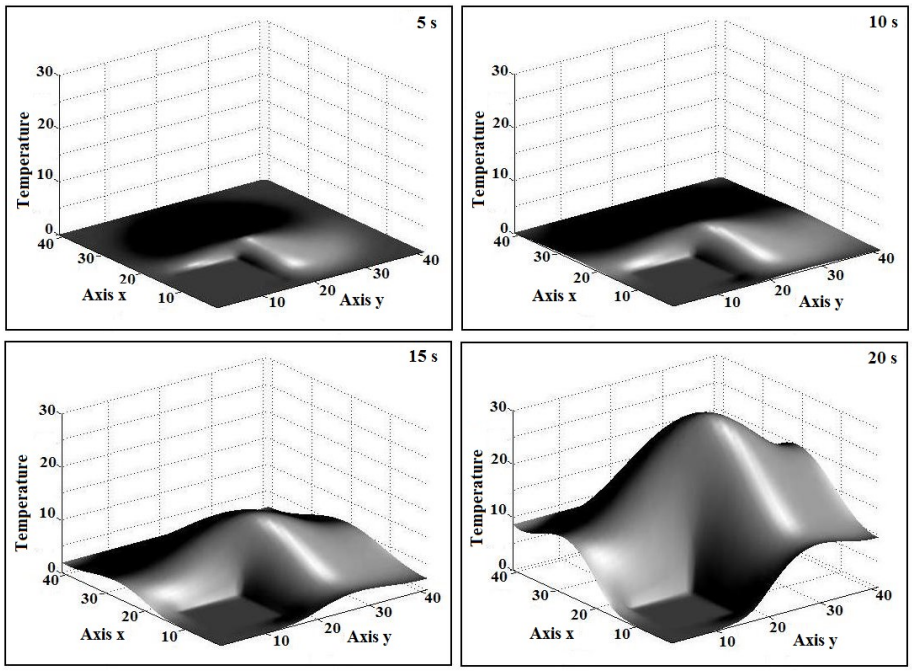

Fig. 2. Results of the study of the quasilinear model of heat transfer in a plate with a zone of anomalous thermal conductivity.

When simulating the process, it was assumed that there was a mass source located on one of the plate boundaries. The source maintained a constant concentration of the substance, equal to 1 conventional unit. The model assumed that there is no mass transfer with the environment.

In order to make the problem less trivial, we introduce the following complication. Let us assume that the investigated plate contains a kind of obstacle - a non-conductive area with a zero diffusion coefficient. The results of the model experiment are shown in Figure 3. The applicate axis is the concentration in arbitrary units.

The results obtained make it possible to investigate the distribution of matter in an object containing areas that impede the normal course of the process.

4 Discussion

The presented examples illustrate the possibilities of a discrete approach to modeling transport processes using cellular automata systems. The results obtained in all cases correspond to the generally accepted ideas about the nature and course of the

processes under consideration. It should be noted that the same program was used to simulate both thermal conductivity and diffusion. The latter follows from the physical analogy of processes obeying the gradient laws of the connection between the transferred potential and the flows of substance.

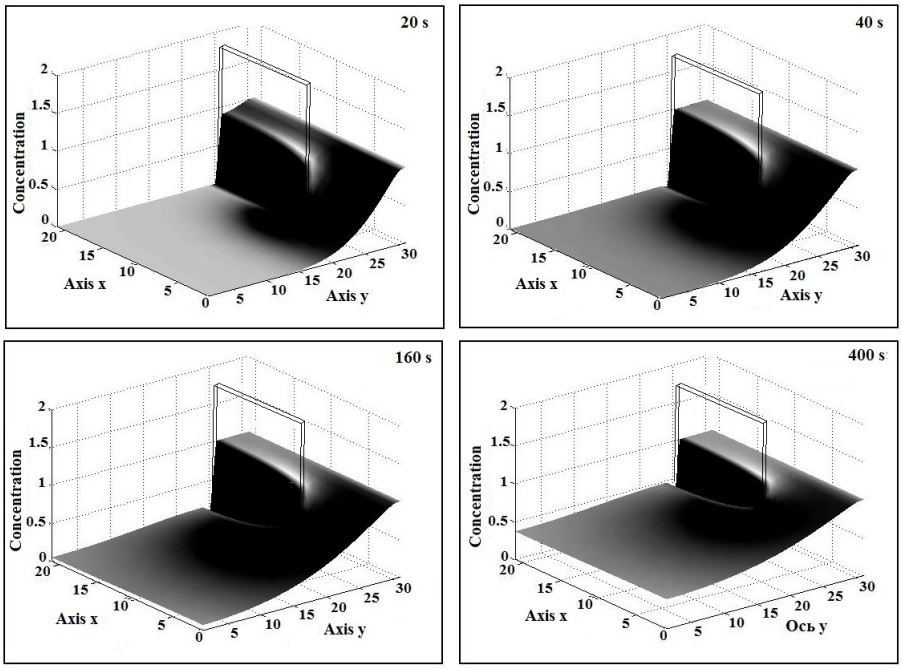

Fig. 3. Results of modeling the diffusion of matter in a plate with an obstacle.

Equally important is the fact that when moving from one example to another, the simulator underwent very minimal changes. Only the dependencies were changed, according to which the parameters of the sources, the characteristics of the material were calculated, and, if necessary, the coordinates of the anomalous zones were introduced.

The convenience of using discrete approaches to simulate and analyze various technological processes was noted by a number of authors [12-15]. At the same time, it was pointed out that these approaches allow avoiding many of the difficulties inherent in classical methods, which are mentioned above in this article.

5 Conclusion

The approach based on systems of cellular automata makes it possible to create effective models for the study of dynamic spatial phenomena, in particular, the processes of molecular transfer of substances. Models based on cellular automata

make it possible to study processes in inhomogeneous media in a nonlinear and non-uniform setting.

The use of cellular automata systems for the analysis of complex technological processes can be recommended. In this case, the physical essence of the problem becomes extremely clear and logically correct. It should be said that this statement is true not only for systems of cellular automata, but also for most other research methods that imply the sampling of space according to a functional feature.

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